

This Page Is Inserted by IFW Operations
and is not a part of the Official Record

BEST AVAILABLE IMAGES

Defective images within this document are accurate representations of the original documents submitted by the applicant.

Defects in the images may include (but are not limited to):

- BLACK BORDERS
- TEXT CUT OFF AT TOP, BOTTOM OR SIDES
- FADED TEXT
- ILLEGIBLE TEXT
- SKEWED/SLANTED IMAGES
- COLORED PHOTOS
- BLACK OR VERY BLACK AND WHITE DARK PHOTOS
- GRAY SCALE DOCUMENTS

IMAGES ARE BEST AVAILABLE COPY.

**As rescanning documents *will not* correct images,
please do not report the images to the
Image Problem Mailbox.**

THIS PAGE BLANK (USPTO)

(19) World Intellectual Property Organization
International Bureau



(43) International Publication Date
30 August 2001 (30.08.2001)

PCT

(10) International Publication Number
WO 01/63244 A1

(51) International Patent Classification⁷: G01N 9/00, 33/48

(74) Agent: ARNOLD, Craig, J.; Amster, Rothstein & Ebenstein, 90 Park Avenue, New York, NY 10016 (US).

(21) International Application Number: PCT/US01/05150

(81) Designated States (*national*): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW.

(22) International Filing Date: 16 February 2001 (16.02.2001)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
09/514,026 25 February 2000 (25.02.2000) US

(84) Designated States (*regional*): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

(71) Applicant: AMERICAN HOME PRODUCTS CORPORATION [US/US]; Five Giralda Farms, Madison, NJ 07940-0874 (US).

Published:

- with international search report
- before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.



(72) Inventors: CHEN, James, M.; 7 Sgt. David Stoddard Court, Bedminster, NJ 07921 (US). MOBILIO, Dominick; 35 Sneider Road, Warren, NJ 07059 (US). MOY, Franklin, J.; 37 Burch Street, Arlington, MA 02414 (US). PARRIS, Kevin, D.; 112 Woodbine Street, Auburndale, MA 02466 (US). POWERS, Robert; 3 Magnolia Drive, Westford, MA 01866 (US). BAO XU, Zhang; 40 Fieldston Circle, Tewksbury, MA 01876 (US).

WO 01/63244 A1

(54) Title: SOLUTION AND CRYSTAL STRUCTURES OF MMP-13 ACTIVE SITE AND USES THEREOF

(57) Abstract: The present invention relates to the three dimensional structure of human collagenase 3 (MMP-13), as well as to (i) methods of using the MMP-13 structure to rationally design or identify compounds or molecules that inhibit or activate MMP-13 activity, and (ii) compounds identified using said methods.

USSN: 10/071073 FILED: 02/8/02
A0000518-01-CFP

SOLUTION AND CRYSTAL STRUCTURES OF MMP-13 ACTIVE SITE AND USES THEREOF

5 **Field of the Invention**

The present invention relates to the three dimensional structure of human collagenase 3 (MMP-13), as well as to (i) methods of using the MMP-13 structure to rationally design or identify compounds or molecules that inhibit or activate MMP-13 activity, and (ii) compounds identified using said methods.

10

Background of the Invention

Human collagenase-3 (MMP-13) is a member of the matrix metalloproteinase (MMP) family which includes the collagenases, stromelysins and gelatinases. The MMPs are involved in the degradation of the extracellular matrix and are associated with normal tissue remodeling processes such as pregnancy, wound healing, and angiogenesis. MMP expression and activity is highly controlled because of the degradative nature of these enzymes, where an apparent loss in MMP regulation results in the pathological destruction of connective tissue and the ensuing disease state. Accordingly, MMPs are a highly active set of targets for the design of therapeutic agents for the disease areas of arthritis and oncology (for reviews, see Woessner, J. F., FASEB 1991; Ries, C., and Petrides, E., Biol. Chem. Hoppe-Seyler 1995; Browner, M. F., Perspect. Drug Discovery Des. 1995; Morphy, *et al.*, Curr. Med. Chem. 1995; and Zask, *et al.*, Curr. Pharm. Des. 1996).

25 MMP-13 was identified on the basis of differential expression in normal breast tissues and in breast carcinoma. In addition, its expression has been reported in squamous cell carcinomas of the larynx, head and neck, in HCS-2/8 human chondrosarcoma cells, during fetal ossification, and in articular cartilage of arthritic patients.

30 There have been a number of X-ray and NMR structures solved for
the catalytic domain of MMPs complexed with a variety of inhibitors (see *e.g.*,
Bode, *et al.*, EMBO J. 1994; Gooley, *et al.*, Nat. Struct. Biol. 1994; Lovejoy, *et*
al., Science 1994; Lovejoy, *et al.*, Ann. N. Y. Acad. Sci. 1994; Lovejoy, *et al.*,

Biochemistry 1994; Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994; Stams, *et al.*, Nat. Struct. Biol. 1994; Becker, *et al.*, Protein Sci. 1995; Gonnella, *et al.*, Proc. Natl. Acad. Sci. U.S.A. 1995; Van Doren, *et al.*, Protein Sci. 1995; Botos, *et al.*, Proc. Natl. Acad. Sci. USA 1996; Broutin, *et al.*, Acta Crystallogr., Sect. D: Biol. Crystallogr. 1996; Gooley, *et al.*, J. Biomol. NMR 1996; Betz, *et al.*, Eur. J. Biochem. 1997; Gonnella, *et al.*, Bioorg. Med. Chem. 1997; and Moy, *et al.*, Biochemistry 1998). There is a close similarity in the overall three-dimensional fold for these proteins consistent with the relatively high sequence homology (> 40%). Despite this similarity in the MMP structures, there is a distinct substrate specificity between these enzymes indicative of specific biological roles for the various MMPs and a corresponding association with unique disease processes. One example of this potential specificity is the over-expression of MMP-13 in breast carcinoma and MMP-1 in papillary carcinomas. Therefore, the current paradigm in the development of MMP inhibitors is to design specificity into the structures of the small molecule instead of developing a broad spectrum MMP inhibitor (Birkedal-Hansen, *et al.*, Crit. Rev. Oral Biol. Med. 1993; and Rockwell, *et al.*, J. Am. Chem. Soc. 1996). The rationale behind this approach is that an inhibitor specific for the MMP uniquely associated with a disease process may potentially minimize toxic side effects. Therefore, extensive structural information for the various MMPs is critical for a structure-based approach in designing inhibitor selectivity (Birkedal-Hansen, *et al.*, Crit. Rev. Oral Biol. Med. 1993; Rockwell, *et al.*, J. Am. Chem. Soc. 1996; Ghose, *et al.*, J. Am. Chem. Soc. 1995; Hajduk, *et al.*, J. Am. Chem. Soc. 1997; and Olejniczak, *et al.*, J. Am. Chem. Soc. 1997).

This concept has been facilitated by the extensive structural data available for the MMPs where a significant difference in the size and shape of the S1' pocket has been observed (Moy, *et al.*, Biochemistry 1998; Bode, *et al.*, EMBO J. 1994; Gooley, *et al.*, Nat. Struct. Biol. 1994; Lovejoy, *et al.*, Ann. N.Y. Acad. Sci. 1994; Lovejoy, *et al.*, Biochemistry 1994; Lovejoy, *et al.*, Science 1994; Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994; Stams, *et al.*, Nat. Struct. Biol. 1994; Becker, *et al.*, Protein Sci. 1995; Gonnella, *et al.*, Proc. Natl.

-3-

Acad. Sci. U.S.A. 1995; Van Doren, *et al.*, Protein Sci. 1995; Botos, *et al.*, Proc. Natl. Acad. Sci. U.S.A. 1996; Broutin, *et al.*, Acta Crystallogr., Sect. D: Biol. Crystallogr. 1996; Gooley, *et al.*, J. Biomol. NMR 1996; Betz, *et al.*, Eur. J. Biochem. 1997; and Gonnella, *et al.*, Bioorg. Med. Chem. 1997). This structural
5 difference across the MMP family provides an obvious approach for designing specificity into potent MMP inhibitors by designing compounds that appropriately fill the available space in the S1' pocket while taking advantage of sequence differences. A number of examples have been previously reported using this approach where some selectivity between MMPs has been achieved by
10 incorporating a biphenyl into the S1' pocket (*see e.g.*, Hajduk, *et al.*, J. Am. Chem. Soc. 1997; and Olejniczak, *et al.*, J. Am. Chem. Soc. 1997).

The inventors have determined both the solution and crystal structures of MMP-13, and, using rational drug design methods, have designed a novel, potent inhibitor that is highly selective for MMP-13.

15

Summary of the Invention

The present invention relates to the three dimensional structure of human collagenase 3 (MMP-13), and more specifically, to the crystal and solution structures of MMP-13 complexed with the inhibitor N-Hydroxy-2-[(4-methoxy-benzenesulfonyl)-pyridin-3-ylmethyl-amino]-3-methyl-benzamide
20 (hereinafter referred to as "Compound A"), as determined using crystallography, spectroscopy and various computer modeling techniques. Particularly, the invention is directed to an MMP-13 active site comprised of the three dimensional structures of various binding pockets located both to the right (S1',
25 S2', S3') and left (S1, S2, S3) of the catalytic zinc of MMP-13, and most particularly is directed to the three dimensional structure of an MMP-13 active site comprising the catalytic zinc and the S1' binding pocket, which is critical to the design and selection of inhibitors with increased potency and specificity for MMP-13, or conversely, for the design and selection of inhibitors of matrix
30 metalloproteinases that are specific against MMP-13.

Accordingly, the present invention discloses a solution comprising a biologically active catalytic fragment of human collagenase-3 (MMP-13) complexed with Compound A, as well as a crystallized catalytic fragment of MMP-13 complexed with Compound A. The three dimensional structure of the catalytic fragment of MMP-13 is provided by the relative atomic structural coordinates of Figure 4, as obtained from spectroscopy data, and Figure 5, as obtained from crystallography data. Also provided is an active site of MMP-13, characterized by a catalytic zinc, a beta strand, a Ca^{2+} binding loop, an alpha helix and a random coil region, wherein the beta strand of said active site preferably comprises residues N14, L15, T16, Y17, R18, I19, and V20 according to Figure 1; the Ca^{2+} binding loop comprises residues F75, D76, G77, P78, and S79 according to Figure 1, the alpha helix comprises residues N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, and H123 according to Figure 1, and the random coil region comprises residues P139, I140, and Y141 according to Figure 1. Said active site is further characterized by a three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, \pm a root mean square deviation from the catalytic zinc and conserved backbone atoms of said amino acids of not more than 1.5\AA .

In an alternate embodiment of the invention, an active site of MMP-13 is characterized by a three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, \pm a root mean square deviation from the catalytic zinc and conserved backbone atoms of said amino acids of not more than 1.5\AA .

The solution or crystal structural coordinates of MMP-13 or portions thereof as provided by this invention may be stored in a

machine-readable form on a machine-readable storage medium, e.g. a computer hard drive, diskette, DAT tape, etc., for display as a three-dimensional shape or for other uses involving computer-assisted manipulation of, or computation based on, the structural coordinates or the three-dimensional structures they

5 define. By way of example, the data defining the three dimensional structure of MMP-13 or an MMP-13 complex of the present invention, or of a portion of MMP-13 or an MMP-13 complex as disclosed herein, may be stored in a machine-readable storage medium, and may be displayed as a graphical three-dimensional representation of the relevant structural coordinates, typically

10 using a computer capable of reading the data from said storage medium and programmed with instructions for creating the representation from such data.

Accordingly, the present invention provides a machine, such as a computer, programmed in memory with the coordinates of the MMP-13 molecule or molecular complex, or portions thereof (such as, by way of

15 example, the coordinates of the MMP-13 catalytic zinc with adjacent S1', S2' and/or S3' binding pockets), together with a program capable of converting the coordinates into a three dimensional graphical representation of the structural coordinates on a display connected to the machine. A machine having a memory containing such data aids in the rational design or selection of

20 inhibitors or activators of MMP-13 activity, including the evaluation of ability of a particular chemical entity to favorably associate with MMP-13 or an MMP-13 complex as disclosed herein, as well as in the modeling of compounds, proteins, complexes, etc. related by structural or sequence homology to MMP-13.

The present invention is additionally directed to a method of

25 determining the three dimensional structure of a molecule or molecular complex whose structure is unknown, comprising the steps of first obtaining crystals or a solution of the molecule or molecular complex whose structure is unknown, and then generating X-ray diffraction data from the crystallized molecule or molecular complex and/or generating NMR data from the solution of the

30 molecule or molecular complex. The generated diffraction or spectroscopy data from the molecule or molecular complex can then be compared with the known

three dimensional structure of MMP-13 as disclosed herein, and the three dimensional structure of the unknown molecule or molecular complex conformed to the known MMP-13 structure using standard techniques such as molecular replacement analysis, 2D, 3D and 4D isotope filtering, editing and
5 triple resonance NMR techniques, and computer homology modeling. Alternatively, a three dimensional model of the unknown molecule may be generated by generating a sequence alignment between MMP-13 and the unknown molecule, based on any or all of amino acid sequence identity, secondary structure elements or tertiary folds, and then generating by computer
10 modeling a three dimensional structure for the molecule using the three dimensional structure of, and sequence alignment with, MMP-13.

The present invention further provides a method for identifying a potential inhibitor or activator of MMP-13, comprising the steps of using a three dimensional structure of MMP-13 as defined by the relative structural
15 coordinates of amino acids encoding MMP-13 to design or select a potential inhibitor or activator, and synthesizing or obtaining said potential inhibitor or activator. The inhibitor or activator may be selected by screening an appropriate database, may designed *de novo* by analyzing the steric configurations and charge potentials of an empty MMP-13 active site in
20 conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors or activators to MMP-13 or other collagenases in order to create "hybrid" activators or inhibitors. The method of the present invention is preferably used to design or select inhibitors of MMP-13 activity.

25 Alternatively, the present invention provides a method for identifying a potential inhibitor or activator that is selective for one or more members of the matrix metalloproteinase family except MMP-13, comprising the steps of (i) using the three dimensional structures of MMP-13 and the desired target matrix metalloproteinase(s) as defined by the relative structural
30 coordinates of amino acids encoding MMP-13 and the target matrix metalloproteinase(s) in order to design or select such a potential inhibitor or

-7-

activator, and (ii) synthesizing or obtaining said potential inhibitor or activator. In this case, the potential inhibitor or activator is designed to incorporate chemical or steric features favorable for association with an active site of the desired matrix metalloproteinase(s) and unfavorable for association with an MMP-13 active site, preferably where said active site comprises the MMP-13 S1' pocket. The inhibitor or activator may be selected by screening an appropriate database, may be designed *de novo* by analyzing the steric configurations and charge potentials of empty MMP-13/matrix metalloproteinase active sites in conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors or activators to MMP-13 or other collagenases in order to create "hybrid" activators or inhibitors.

Also provided by the present invention are the inhibitors and activators designed or selected using the methods disclosed herein.

Brief Description of the Figures

Figure 1 depicts the amino acid sequence encoding the catalytic fragment of human MMP-13.

Figure 2 depicts the sequence based alignment between (A) MMP-13 and MMP-8 and (B) MMP-13 and MMP-1 used for the MMP-13 homology model.

Figure 3 is an illustration of the sulfonamide derivative of the hydroxamic inhibitor N-Hydroxy-2-[(4-methoxy-benzenesulfonyl)-pyridin-3-ylmethyl-amino]-3-methyl-benzamide (Compound A), with the corresponding proton labels.

Figure 4 lists the atomic structure coordinates for the restrained minimized mean structure of MMP-13 complexed with Compound A as derived by NMR spectroscopy. "Atom type" refers to the atom whose coordinates are being measured. "Residue" refers to the type of residue of which each measured atom is a part - i.e., amino acid, cofactor, ligand or solvent. The "x, y and z" coordinates indicate the Cartesian coordinates of each measured atom's location

-8-

(Å). All non-protein atoms (Compound A, zinc and calcium) are listed as HETATM instead of atoms using PDB conventions.

Figure 5 lists the atomic structure coordinates for MMP-13 as derived by X-ray diffraction of a crystallized MMP-13:Compound A complex.

- 5 Figure headings are as noted above, except "Occ" indicates the occupancy factor, and "B" indicates the "B-value", which is a measure of how mobile the atom is in the atomic structure (Å²). "MOL" indicates the segment identification used to uniquely identify each molecule in the crystal.

- Figure 6 is an illustration of the Compound B inhibitor, with the
10 corresponding proton labels.

- Figure 7 is a design scheme dividing 2-[Benzyl-(4-phenethyloxy-benzenesulfonyl)-amino]-N-hydroxy-3,5-dimethyl-benzamide (hereinafter referred to as "Compound C") into two components corresponding to its potency component (2-[Benzyl-(4-methoxy-benzenesulfonyl)-amino]-N-hydroxy-3,5-
15 dimethyl-benzamide, hereinafter referred to as "Compound D") and its selectivity component, thereby providing the basis for the design of a hybrid inhibitor with Compound B.

- Figure 8A is a design scheme showing the flow from Compound B and Compound C to the hybrid inhibitor benzofuran-2-carboxylic acid (2-{4-
20 [benzyl-(2-hydroxycarbamoyl-4,6-dimethyl-phenyl)-sulfamoyl]-phenoxy}-ethyl)-amide (hereinafter referred to as "Compound E"). Figure 8B illustrates an expanded view of the NMR MMP-13:Compound B complex overlaid with the MMP-13:Compound D model, demonstrating the approach to forming the hybrid inhibitor Compound E. The MMP-13 active site is shown as a grid
25 surface with Compound B and Compound D shown as liquorice bonds. The view is looking at the S1' pocket.

Detailed Description of the Invention

As used herein, the following terms and phrases shall have the meanings set forth below:

“Compound A” is N-Hydroxy-2-[(4-methoxy-benzenesulfonyl)-pyridin-3-ylmethyl-amino]-3-methyl-benzamide, as shown in Figure 3.

“Compound B” is the compound having the chemical structure shown in Figure 6. “Compound C” is 2-[Benzyl-(4-phenethyloxy-benzenesulfonyl)-amino]-N-hydroxy-3,5-dimethyl-benzamide, as shown in Figure 7. “Compound D” is 2-[Benzyl-(4-methoxy-benzenesulfonyl)-amino]-N-hydroxy-3,5-dimethyl-benzamide, also shown in Figure 7. “Compound E” is Benzofuran-2-carboxylic acid (2-{4-[benzyl-(2-hydroxycarbamoyl-4,6-dimethyl-phenyl)-sulfamoyl]-phenoxy}-ethyl)-amide, as shown in Figure 8A. “Compound F” is 2-(Benzyl-4-(3-phenyl-propoxy)-benzenesulfonyl)-amino)-N-hydroxy-3,5-dimethyl-benzamide.

Unless otherwise noted, “MMP-13” includes both human collagenase 3 as encoded by the amino acid sequence of Figure 1 (including conservative substitutions thereof), as well as “MMP-13 analogues”, defined herein as proteins comprising an MMP-13 like active site as defined by the present invention, including, but not limited to, an active site characterized by a three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, \pm a root mean square deviation from the catalytic zinc and conserved backbone atoms of said amino acids of not more than 1.5Å, or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å. Alternatively, an MMP-13 analogue of the present invention is a protein which comprises an MMP-13 like active site characterized by a catalytic zinc, a beta strand, a Ca^{2+} binding loop, an alpha helix and a random coil region, or, more particularly, comprising an active site characterized by a three dimensional structure comprising the relative structural coordinates of the catalytic zinc and of amino acid residues N14, L15, T16, Y17, R18, I19, V20,

-10-

F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to Figures 4 or 5, or more preferably, where said three dimensional structure further comprises the relative structural coordinates of amino acid residues G80, L81, L82, A83, H84, 5 A85, K109, G110, Y111, S124, L125, G126, L127, D128, H129, S130, K131, D132, P133, G134, A135, L136, M137, F138, T142, Y143, T144, and G145 according to Figures 4 or 5, or most preferably, where said three dimensional structure still further comprises the relative structural coordinates of F149 and P152 according to Figures 4 or 5, in each case, \pm a root mean square deviation 10 from the catalytic zinc and the conserved backbone atoms (N, C α , C, and O) of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å).

Unless otherwise indicated, "protein" or "molecule" shall include a protein, protein domain, polypeptide or peptide.

15 "Structural coordinates" are the Cartesian coordinates corresponding to an atom's spatial relationship to other atoms in a molecule or molecular complex. Structural coordinates may be obtained using x-ray crystallography techniques or NMR techniques, or may be derived using molecular replacement analysis or homology modeling. Various software 20 programs allow for the graphical representation of a set of structural coordinates to obtain a three dimensional representation of a molecule or molecular complex. The structural coordinates of the present invention may be modified from the original sets provided in Figures 4 or 5 by mathematical manipulation, such as by inversion or integer additions or subtractions. As 25 such, it is recognized that the structural coordinates of the present invention are relative, and are in no way specifically limited by the actual x, y, z coordinates of Figures 4 and 5. Further, it is recognized that the structural coordinates taken from Figure 5 may be from either molecule of MMP-13 catalytic fragment in the MMP-13:Compound A crystal (i.e., from A-13 or B-13).

30 An "agent" shall include a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibiotic or drug.

-11-

“Root mean square deviation” is the square root of the arithmetic mean of the squares of the deviations from the mean, and is a way of expressing deviation or variation from the structural coordinates described herein.

It will be obvious to the skilled practitioner that the numbering of the amino acid residues in the various isoforms of MMP-13 or in MMP-13 analogues covered by the present invention may be different than that set forth herein, or may contain certain conservative amino acid substitutions that yield the same three dimensional structures as those defined by Figures 4 or 5 herein. Corresponding amino acids and conservative substitutions in other isoforms or analogues are easily identified by visual inspection of the relevant amino acid sequences or by using commercially available homology software programs. “Conservative substitutions” are those amino acid substitutions which are functionally equivalent to the substituted amino acid residue, either by way of having similar polarity, steric arrangement, or by belonging to the same class as the substituted residue (e.g., hydrophobic, acidic or basic), and includes substitutions having an inconsequential effect on the three dimensional structure of MMP-13 with respect to the use of said structure for the identification and design of MMP-13 activators or inhibitors, for molecular replacement analyses and/or for homology modeling.

An “active site” refers to a region of a molecule or molecular complex that, as a result of its shape and charge potential, favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibiotic or drug). As such, the active site may include both the actual site of substrate cleavage or collagenase activity, as well as certain or all binding sites or pockets adjacent to the site of substrate cleavage that nonetheless may affect MMP-13 activity upon interaction or association with an agent, either by direct interference with the site of substrate cleavage or by indirectly affecting the steric conformation or charge potential of the MMP-13 molecule. The catalytic center of the MMP-13 molecule is characterized by a zinc atom chelated by H119, H123 and H129. MMP-13 binding sites or pockets located to the right of

-12-

the catalytic zinc include S1', S2' and S3'. Binding sites or pockets to the left of the catalytic zinc include S1, S2 and S3.

The present invention relates to the three dimensional structure of human collagenase 3 (MMP-13) or an MMP-13 analogue, and more specifically, to the crystal and solution structures of MMP-13 complexed with an inhibitor, referred to herein as "Compound A", as determined using crystallography, spectroscopy and various computer modeling techniques. The three dimensional solution and crystal structures of the MMP-13:Compound A complex (as disclosed herein at Figures 4 or 5, respectively) and the uncomplexed MMP-13 catalytic fragment (which may be computationally derived from the structural coordinates of Figures 4 or 5) are useful for a number of applications, including, but not limited to, the visualization, identification and characterization of MMP-13 active sites, including the MMP-13 catalytic zinc chelated by H119, H123 and H129, as well as the various MMP-13 binding pockets adjacent to the catalytic zinc of the MMP-13 molecule. The active site structures may then be used to predict the orientation and binding affinity of a designed or selected activator or inhibitor of the MMP-13 protein. Accordingly, the invention is particularly directed to the three dimensional structure of an MMP-13 active site, including but not limited to the S1', S2', S3', S1, S2 and/or S3 binding pockets, taken separately or together with the catalytic zinc of the MMP-13 molecule.

The present invention provides a solution comprising a biologically active catalytic fragment of human collagenase-3 (MMP-13) complexed with Compound A. In a particular embodiment, the catalytic fragment of MMP-13 comprises the amino acid residues of Figure 1, or conservative substitutions thereof. Preferably, the solution provided for herein comprises MMP-13 complexed with Compound A in a 1:1 molar ratio, and more preferably comprises 1 mM MMP-13 in an equimolar complex with Compound A, in a buffer comprising 10mM deuterated Tris-Base, 100mM NaCl, 5mM CaCl₂, 0.1mM ZnCl₂, 2mM NaN₃, and 10 mM deuterated DTT in either 90% H₂O/10% D₂O or 100% D₂O, at a preferred pH of 6.5. The concentration of

-13-

MMP-13:Compound A in the solution should be high enough to yield a good signal-to-noise ratio in the NMR spectrum, but not so high as to result in precipitation or aggregation of the protein. Further, the MMP-13 of the solution may be either ^{15}N enriched or ^{15}N , ^{13}C enriched. As exemplified below, NMR spectra from the solution of the present invention are preferably obtained at a temperature of 35°C.

The secondary structure of the catalytic fragment used in the solution of the present invention comprises three alpha helices and a mixed parallel and anti-parallel beta sheet comprising five beta strands, configured in the order β_I , α_A , β_{II} , β_{III} , β_{IV} , β_V , α_B , and α_C . The three alpha helices correspond to residues 28-44 (α_A), 112-123 (α_B) and 153-163 (α_C) of Figure 1, and the five beta strands correspond to residues 83-86 (β_I), 95-100 (β_{II}), 59-66 (β_{III}), 14-20 (β_{IV}), and 49-53 (β_V) of Figure 1, respectively. While the solution of the present invention comprises MMP-13 in a 1:1 molar ratio with Compound A, it is understood that one of ordinary skill in the art may devise additional solutions using alternate inhibitors or ligands in the appropriate molar concentrations, thereby preventing the auto-degradation of MMP-13 and creating a solution of sufficient stability and concentration to obtain a usable NMR spectrum.

The protein used in the solution of the present invention includes MMP-13, as well as MMP-13 analogues, where said protein comprises an active site characterized by the three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 (or conservative substitutions thereof) according to the solution coordinates of Figure 4, \pm a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å, or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å. These residues comprise the residues most closely associated with Compound A in the MMP-13:Compound A complex, as determined from the observed NOEs between MMP-13 and Compound A (Table 1).

Alternatively, a protein used in the solution of the present invention comprises an active site characterized by a catalytic zinc, a beta strand (comprising amino acid residues N14, L15, T16, Y17, R18, I19, and V20 or conservative substitutions thereof), a Ca^{2+} binding loop (comprising amino acid residues F75, D76, G77, P78, and S79 or conservative substitutions thereof), an alpha helix (comprising amino acid residues N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, and H123 or conservative substitutions thereof) and a random coil region (comprising amino acid residues P139, I140, and Y141 or conservative substitutions thereof), or, more particularly,

characterized by a three dimensional structure comprising the relative structural coordinates of the catalytic zinc and the amino acid residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to Figure 4, or more preferably, where said three dimensional structure further comprises the relative structural coordinates of amino acid residues G80, L81, L82, A83, H84, A85, K109, G110, Y111, S124, L125, G126, L127, D128, H129, S130, K131, D132, P133, G134, A135, L136, M137, F138, T142, Y143, T144, and G145 according to Figure 4 (incorporating an S1' pocket in the active site), or most preferably, where said three dimensional structure still further comprises the relative structural coordinates of F149 and P152 according to Figure 4 (further defining a hydrophobic area at the bottom of the S1' pocket), including, in each case, conservative substitutions of said amino acids and, in each case, \pm a root mean square deviation from the catalytic zinc and the conserved backbone atoms (N, $\text{C}\alpha$, C, and O) of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å). Finally, in the most preferred embodiment, the protein used in the solution of the present invention comprises the complete structural coordinates according to Figure 4, \pm a root mean square deviation from the conserved backbone atoms of said amino acids (or conservative substitutions thereof) of not more than 1.5Å (or more preferably, not more than 1.0Å, and most preferably, not more than 0.5Å).

-15-

Also provided by the present invention is a crystallized catalytic fragment of MMP-13 complexed with Compound A. The crystal of the present invention effectively diffracts X-rays for the determination of the structural coordinates of the MMP-13:Compound A complex, and is characterized as being
5 in orthorhombic form with space group P21212, and having unit cell parameters of $a=108.3\text{\AA}$, $b=79.8\text{\AA}$, and $c=36.1\text{\AA}$. Further, the crystal complex of the present invention consists of two molecules of MMP-13:Compound A complex in the asymmetric crystal unit.

In a preferred embodiment, the MMP-13 of the crystal complex of
10 the present invention comprises the amino acid residues of Figure 1 (or conservative substitutions thereof), and is characterized by a secondary structure comprising three alpha helices and a mixed parallel and anti-parallel beta sheet comprising five beta strands, configured in the order β_I , α_A , β_{II} , β_{III} , β_{IV} , β_V , α_B , and α_C . Further, the three alpha helices preferably correspond to
15 residues 28-44 (α_A), 112-123 (α_B) and 153-163 (α_C) of Figure 1, and the five beta strands correspond to residues 83-86 (β_I), 95-100 (β_{II}), 59-66 (β_{III}), 14-20 (β_{IV}), and 49-53 (β_V) of Figure 1, respectively.

The protein used in the crystal or crystal complex of the present invention includes MMP-13, as well as MMP-13 analogues, where said protein
20 comprises an active site characterized by the three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 (or conservative substitutions thereof) according to the crystal coordinates of Figure 5, \pm a root mean square deviation from the catalytic zinc and the conserved backbone
25 atoms of said amino acids of not more than 1.5\AA , or more preferably, not more than 1.0\AA , or most preferably, not more than 0.5\AA .

Alternatively, a protein used in the crystal or crystal complex of the present invention comprises an active site characterized by a catalytic zinc, a beta strand (comprising amino acid residues N14, L15, T16, Y17, R18, I19, and
30 V20 or conservative substitutions thereof), a Ca^{2+} binding loop (comprising amino acid residues F75, D76, G77, P78, and S79 or conservative substitutions

-16-

thereof), an alpha helix (comprising amino acid residues N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, and H123 or conservative substitutions thereof) and a random coil region (comprising amino acid residues P139, I140, and Y141 or conservative substitutions thereof), or, more particularly, characterized by a three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to Figure 5, or more preferably, where said three dimensional structure further comprises the relative structural coordinates of amino acid residues G80, L81, L82, A83, H84, A85, K109, G110, Y111, S124, L125, G126, L127, D128, H129, S130, K131, D132, P133, G134, A135, L136, M137, F138, T142, Y143, T144, and G145 according to Figure 5 (incorporating an S1' pocket in the active site), or most preferably, where said three dimensional structure still further comprises the relative structural coordinates of F149 and P152 according to Figure 5 (further defining a hydrophobic area at the bottom of the S1' pocket), in each case, including conservative substitutions of the said amino acids and, in each case, \pm a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å).

Finally, in the most preferred embodiment, the protein used in the crystal of the present invention comprises the complete structural coordinates according to Figure 5, \pm a root mean square deviation from the conserved backbone atoms of said amino acids (or conservative substitutions thereof) of not more than 1.5Å (or more preferably, not more than 1.0Å, and most preferably, not more than 0.5Å).

Molecular modeling methods known in the art may be used to identify an active site or binding pocket of the MMP-13 molecule, MMP-13 molecular complex, or an MMP-13 analogue. Specifically, the structural coordinates provided by the present invention may be used to characterize a

-17-

three dimensional model of the MMP-13 molecule, molecular complex or MMP-13 analogue. From such a model, putative active sites may be computationally visualized, identified and characterized based on the surface structure of the molecule, surface charge, steric arrangement, the presence of reactive amino acids, regions of hydrophobicity or hydrophilicity, etc. Such putative active sites may be further refined using chemical shift perturbations of spectra generated from various and distinct MMP-13 complexes, competitive and non-competitive inhibition experiments, and/or by the generation and characterization of MMP-13 mutants to identify critical residues or characteristics of the active site.

10 The identification of putative active sites of a molecule or molecular complex is of great importance, as most often the biological activity of a molecule or molecular complex results from the interaction between an agent and one or more active sites of the molecule or molecular complex. Accordingly, the active sites of a molecule or molecular complex are the best targets to use in the design or selection of activators or inhibitors that affect the activity of the molecule or molecular complex.

 The present invention is directed to an active site of MMP-13 or an MMP-13 analogue, that, as a result of its shape, reactivity, charge potential, etc., favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibiotic or drug). As such, the active site of the present invention includes both the actual site of substrate cleavage or collagenase activity (the catalytic zinc chelated by H119, H123, and H129), as well as binding sites or pockets adjacent to the site of substrate cleavage (i.e., S1', S2', S3', S1, S2, and/or S3) that may nonetheless affect MMP-13 activity upon interaction or association with an agent, either by direct interference with the site of substrate cleavage or by indirectly affecting the steric conformation or charge potential of the MMP-13 molecule. Accordingly, the present invention is directed to an active site of the MMP-13 molecule characterized by a zinc atom chelated by H119, H123 and H129, and preferably the S1' binding pocket to the right of the catalytic zinc.

-18-

In an alternate embodiment, the active site of the present invention is characterized by the three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 (or conservative substitutions thereof) according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, \pm a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å, or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å.

Alternatively, the active site of the present invention is characterized by a catalytic zinc, a beta strand (comprising amino acid residues N14, L15, T16, Y17, R18, I19, and V20 or conservative substitutions thereof), a Ca^{2+} binding loop (comprising amino acid residues F75, D76, G77, P78, and S79 or conservative substitutions thereof), an alpha helix (comprising amino acid residues N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, and H123 or conservative substitutions thereof) and a random coil region (comprising amino acid residues P139, I140, and Y141 or conservative substitutions thereof), or, more particularly, is characterized by a three dimensional structure comprising the relative solution or crystal structural coordinates of the catalytic zinc and amino acid residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to Figures 4 or 5, respectively, or more preferably, where said three dimensional structure further comprises the relative solution or crystal structural coordinates of amino acid residues G80, L81, L82, A83, H84, A85, K109, G110, Y111, S124, L125, G126, L127, D128, H129, S130, K131, D132, P133, G134, A135, L136, M137, F138, T142, Y143, T144, and G145 according to Figures 4 or 5, or most preferably, where said three dimensional structure still further comprises the relative solution or crystal structural coordinates of F149 and P152 according to Figures 4 or 5, in each case, including conservative substitutions of said amino acids, and in each case, \pm a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å

-19-

(or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å).

In order to use the structural coordinates generated for a crystal or solution structure of the present invention as set forth in Figures 4 and 5, respectively, it is often necessary to display the relevant coordinates as, or convert them to, a three dimensional shape or graphical representation, or to otherwise manipulate them. For example, a three dimensional representation of the structural coordinates is often used in rational drug design, molecular replacement analysis, homology modeling, and mutation analysis. This is typically accomplished using any of a wide variety of commercially available software programs capable of generating three dimensional graphical representations of molecules or portions thereof from a set of structural coordinates. Examples of said commercially available software programs include, without limitation, the following: GRID (Oxford University, Oxford, UK); MCSS (Molecular Simulations, San Diego, CA); AUTODOCK (Scripps Research Institute, La Jolla, CA); DOCK (University of California, San Francisco, CA); Flo99 (Thistlesoft, Morris Township, NJ); Ludi (Molecular Simulations, San Diego, CA); QUANTA (Molecular Simulations, San Diego, CA); Insight (Molecular Simulations, San Diego, CA); SYBYL (TRIPOS, Inc., St. Louis, MO); and LEAPFROG (TRIPOS, Inc., St. Louis, MO).

For storage, transfer and use with such programs, a machine, such as a computer, is provided for that produces a three dimensional representation of the MMP-13 molecule, a portion thereof (such as an active site or a binding site), a MMP-13 molecular complex, or an MMP-13 analogue. The machine of the present invention comprises a machine-readable data storage medium comprising a data storage material encoded with machine-readable data. Machine-readable storage media comprising data storage material include conventional computer hard drives, floppy disks, DAT tape, CD-ROM, and other magnetic, magneto-optical, optical, floptical and other media which may be adapted for use with a computer. The machine of the present invention also comprises a working memory for storing instructions for processing the

-20-

machine-readable data, as well as a central processing unit (CPU) coupled to the working memory and to the machine-readable data storage medium for the purpose of processing the machine-readable data into the desired three dimensional representation. Finally, the machine of the present invention

5 further comprises a display connected to the CPU so that the three dimensional representation may be visualized by the user. Accordingly, when used with a machine programmed with instructions for using said data, e.g., a computer loaded with one or more programs of the sort identified above, the machine provided for herein is capable of displaying a graphical three-dimensional

10 representation of any of the molecules or molecular complexes, or portions of molecules of molecular complexes, described herein.

In one embodiment of the invention, the machine-readable data comprises the relative structural coordinates of the catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 according to Figures 4 or

15 5, in each case, including conservative substitutions thereof, and in each case, \pm a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, and most preferably, not more than 0.5Å), wherein said structural coordinates characterize an active site of MMP-13 or an MMP-13

20 analogue.

In an alternate preferred embodiment, the machine-readable data comprises the structural coordinates of the catalytic zinc and amino acid residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139,

25 I140, and Y141 according to Figures 4 or 5, in each case, including conservative substitutions thereof, and in each case, \pm a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, and most preferably, not more than 0.5Å). In an even more preferred embodiment, the machine-

30 readable data further comprises the relative structural coordinates of amino acid residues G80, L81, L82, A83, H84, A85, K109, G110, Y111, S124, L125, G126,

-21-

L127, D128, H129, S130, K131, D132, P133, G134, A135, L136, M137, F138, T142, Y143, T144, and G145 according to Figures 4 or 5, or most preferably, still further comprises the relative structural coordinates of F149 and P152 according to Figures 4 or 5, in each case, including conservative substitutions of
5 said amino acids, and in each case, \pm a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å).

Finally, it is most preferred that the machine-readable data
10 comprise the relative structural coordinates of all residues constituting the MMP-13 catalytic fragment according to Figures 4 or 5, in each case, \pm a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5Å. In each case, the noted embodiments comprise conservative substitutions of the noted residues resulting in same structural
15 coordinates within the stated root mean square deviation.

The structural coordinates of the present invention permit the use of various molecular design and analysis techniques in order to (i) solve the three dimensional structures of related molecules, molecular complexes or MMP-13 analogues, and (ii) to design, select, and synthesize chemical agents
20 capable of favorably associating or interacting with an active site of an MMP-13 molecule or MMP-13 analogue, wherein said chemical agents potentially act as activators or inhibitors of MMP-13 or of an MMP-13 analogue.

More specifically, the present invention provides a method for determining the molecular structure of a molecule or molecular complex whose
25 structure is unknown, comprising the steps of obtaining crystals or a solution of the molecule or molecular complex whose structure is unknown, and then generating x-ray diffraction data from the crystallized molecule or molecular complex, and/or generating NMR data from the solution of the molecule or molecular complex. The x-ray diffraction data from the molecule or molecular
30 complex whose structure is unknown is then compared to the x-ray diffraction data obtained from the MMP-13:Compound A crystal of the present invention.

-22-

Alternatively, the NMR data from the molecule or molecular structure whose structure is unknown is then compared with the NMR data obtained from the MMP-13:Compound A solution of the present invention. Then, molecular replacement analysis is used to conform the three dimensional structure
5 determined from the MMP-13:Compound A crystal of solution of the present invention to the x-ray diffraction data from the unknown molecule or molecular complex, or, alternatively, 2D, 3D and 4D isotope filtering, editing and triple resonance NMR techniques are used to conform the three dimensional structure determined from the MMP-13:Compound A solution of the present invention to
10 the NMR data from the solution molecule or molecular complex.

Molecular replacement analysis uses a molecule having a known structure as a starting point to model the structure of an unknown crystalline sample. This technique is based on the principle that two molecules which have similar structures, orientations and positions will diffract x-rays similarly. A
15 corresponding approach to molecular replacement is applicable to modeling an unknown solution structure using NMR technology. The NMR spectra and resulting analysis of the NMR data for two similar structures will be essentially identical for regions of the proteins that are structurally conserved, where the NMR analysis consists of obtaining the NMR resonance assignments and the
20 structural constraint assignments, which may contain hydrogen bond, distance, dihedral angle, coupling constant, chemical shift and dipolar coupling constant constraints. The observed differences in the NMR spectra of the two structures will highlight the differences between the two structures and identify the corresponding differences in the structural constraints. The structure
25 determination process for the unknown structure is then based on modifying the NMR constraints from the known structure to be consistent with the observed spectral differences between the NMR spectra.

Accordingly, in one non-limiting embodiment of the invention, the resonance assignments for the MMP-13:Compound A complex provide the
30 starting point for resonance assignments of MMP-13 in a new MMP-13:"unsolved agent" complex. Chemical shift perturbances in two dimensional

-23-

$^{15}\text{N}/^1\text{H}$ spectra can be observed and compared between the MMP-13:Compound A complex and the new MMP-13:agent complex. In this way, the affected residues may be correlated with the three dimensional structure of MMP-13 as provided by the relevant residues of Figure 4. This effectively identifies the region of the MMP-13:agent complex that has incurred a structural change relative to the MMP-13:Compound A complex. The ^1H , ^{15}N , ^{13}C and ^{13}CO NMR resonance assignments corresponding to both the sequential backbone and side-chain amino acid assignments of MMP-13 may then be obtained and the three dimensional structure of the new MMP-13:agent complex may be generated using standard 2D, 3D and 4D triple resonance NMR techniques and NMR assignment methodology, using the MMP-13:Compound A structure, resonance assignments and structural constraints as a reference. Various computer fitting analyses of the new agent with the three dimensional model of MMP-13 may be performed in order to generate an initial three dimensional model of the new agent complexed with MMP-13, and the resulting three dimensional model may be refined using standard experimental constraints and energy minimization techniques in order to position and orient the new agent in association with the three dimensional structure of MMP-13.

The present invention further provides that the structural coordinates of the present invention may be used with standard homology modeling techniques in order to determine the unknown three-dimensional structure of a molecule or molecular complex. Homology modeling involves constructing a model of an unknown structure using structural coordinates of one or more related protein molecules, molecular complexes or parts thereof (i.e., active sites). Homology modeling may be conducted by fitting common or homologous portions of the protein whose three dimensional structure is to be solved to the three dimensional structure of homologous structural elements in the known molecule, specifically using the relevant (i.e., homologous) structural coordinates provided by Figures 4 and/or 5 herein. Homology may be determined using amino acid sequence identity, homologous secondary structure elements, and/or homologous tertiary folds. Homology modeling can

-24-

include rebuilding part or all of a three dimensional structure with replacement of amino acids (or other components) by those of the related structure to be solved.

Accordingly, a three dimensional structure for the unknown
5 molecule or molecular complex may be generated using the three dimensional structure of the MMP-13:Compound A complex of the present invention, refined using a number of techniques well known in the art, and then used in the same fashion as the structural coordinates of the present invention, for instance, in applications involving molecular replacement analysis, homology modeling, and
10 rational drug design.

Determination of the three dimensional structure of MMP-13 and its catalytic active site as disclosed herein is critical to the rational identification and/or design of therapeutic agents that may act as inhibitors or activators of MMP-13 enzymatic activity. Alternatively, using conventional drug assay
15 techniques, the only way to identify such an agent is to screen thousands of test compounds, either in culture or by administration to suitable animal models in a laboratory setting, until an agent having the desired inhibitory or activating effect on a target compound is identified. Necessarily, such conventional screening methods are expensive, time consuming, and do not elucidate the
20 method of action of the identified agent on the target compound.

However, advancing X-ray, spectroscopic and computer modeling technologies allow researchers to visualize the three dimensional structure of a targeted compound. Using such a three dimensional structure, researchers identify putative binding sites and then identify or design agents to interact with
25 these binding sites. These agents are then screened for an activating or inhibitory effect upon the target molecule. In this manner, not only are the number of agents to be screened for the desired activity greatly reduced, but the mechanism of action on the target compound is better understood.

Accordingly, the present invention further provides a method for
30 identifying a potential inhibitor or activator of MMP-13, comprising the steps of using a three dimensional structure of MMP-13 as defined by the relative

-25-

structural coordinates of amino acids encoding MMP-13 to design or select a potential inhibitor or activator, and synthesizing or obtaining said potential inhibitor or activator. The inhibitor or activator may be selected by screening an appropriate database, may designed *de novo* by analyzing the steric configurations and charge potentials of an empty MMP-13 active site in conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors or activators to MMP-13 or other collagenases in order to create "hybrid" activators or inhibitors. The method of the present invention is preferably used to design or select inhibitors of MMP-13 activity.

An agent that interacts or associates with an active site of MMP-13 or an MMP-13 analogue may be identified by determining an active site of MMP-13 or of the MMP-13 analogue from a three dimensional model of the MMP-13 or MMP-13 analogue, and performing computer fitting analyses to identify an agent which interacts or associates with said active site. Computer fitting analyses utilize various computer software programs that evaluate the "fit" between the putative active site and the identified agent, by (a) generating a three dimensional model of the putative active site of a molecule or molecular complex using homology modeling or the atomic structural coordinates of the active site, and (b) determining the degree of association between the putative active site and the identified agent. The degree of association may be determined computationally by any number of commercially available software programs, or may be determined experimentally using standard binding assays.

Three dimensional models of the putative active site may be generated using any one of a number of methods known in the art, and include, but are not limited to, homology modeling as well as computer analysis of raw structural coordinate data generated using crystallographic or spectroscopy techniques. Computer programs used to generate such three dimensional models and/or perform the necessary fitting analyses include, but are not limited to: GRID (Oxford University, Oxford, UK), MCSS (Molecular Simulations, San Diego, CA), AUTODOCK (Scripps Research Institute, La Jolla,

CA), DOCK (University of California, San Francisco, CA), Flo99 (Thistlesoft, Morris Township, NJ), Ludi (Molecular Simulations, San Diego, CA), QUANTA (Molecular Simulations, San Diego, CA), Insight (Molecular Simulations, San Diego, CA), SYBYL (TRIPOS, Inc., St. Louis, MO) and LEAPFROG (TRIPOS, Inc.,
5 St. Louis, MO).

In a preferred method of the present invention, the identified active site of MMP-13 or the MMP-13 analogue comprises a catalytic zinc, a beta strand, a Ca^{2+} binding loop, an alpha helix and a random coil region. More preferably, the identified active site comprises a catalytic zinc, a beta strand
10 comprising residues N14, L15, T16, Y17, R18, I19, and V20 according to Figure 1 (or conservative substitutions thereof), a Ca^{2+} binding loop comprising residues F75, D76, G77, P78, and S79 according to Figure 1 (or conservative substitutions thereof), an alpha helix comprising residues N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, and H123 according to
15 Figure 1 (or conservative substitutions thereof), and a random coil region comprising residues P139, I140, and Y141 according to Figure 1 (or conservative substitutions thereof).

More specifically, the identified active site of the present method comprises the relative structural coordinates of the catalytic zinc and amino acid
20 residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to Figures 4 or 5, in each case, including conservative substitutions of said amino acids, and in each case, \pm a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said
25 amino acids of not more than 1.5\AA (or more preferably, not more than 1.0\AA , or most preferably, not more than 0.5\AA). In an alternate preferred embodiment, the identified active site further comprises the relative structural coordinates of amino acid residues G80, L81, L82, A83, H84, A85, K109, G110, Y111, S124, L125, G126, L127, D128, H129, S130, K131, D132, P133, G134, A135, L136,
30 M137, F138, T142, Y143, T144, and G145 according to Figures 4 or 5, in each case, including conservative substitutions of said amino acids, and in each case,

-27-

± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å). In yet a third preferred embodiment, the identified active site of the present method further comprises the relative structural coordinates of amino acid residues F149 and P152 according to Figures 4 or 5, in each case, including conservative substitutions of said amino acids, and in each case, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å). Embodiments comprising conservative substitutions of the noted amino acids result in the same structural coordinates of the corresponding residues in Figures 4 or 5 within the stated root mean square deviation.

The effect of such an agent identified by computer fitting analyses on MMP-13 (or MMP-13 analogue) activity may be further evaluated computationally, or experimentally by contacting the identified agent with MMP-13 (or an MMP-13 analogue) and measuring the effect of the agent on the enzyme's activity. Depending upon the action of the agent on the active site of MMP-13, the agent may act either as an inhibitor or activator of MMP-13 activity. Standard enzymatic assays may be performed and the results analyzed to determine whether the agent is an inhibitor of MMP-13 activity (i.e., the agent may reduce or prevent binding affinity between MMP-13 and the relevant substrate, and thereby reduce the level or rate of MMP-13 activity compared to baseline), or an activator of MMP-13 activity (i.e., the agent may increase binding affinity between MMP-13 and the relevant substrate, and thereby increase the level or rate of MMP-13 activity compared to baseline). Further tests may be performed to evaluate the selectivity of the identified agent to MMP-13 with regard to the other metalloproteinases.

Agents designed or selected to interact with MMP-13 must be capable of both physically and structurally associating with MMP-13 *via* various covalent and/or non-covalent molecular interactions, and of assuming a three

-28-

dimensional configuration and orientation that complements the relevant active site of the MMP-13 molecule.

Accordingly, using these criteria, the structural coordinates of the MMP-13:Compound A complex as disclosed herein, and/or structural
5 coordinates derived therefrom using molecular replacement analysis or homology modeling, agents may be designed to increase either or both of the potency and selectivity of known inhibitors or activators, either by modifying the structure of known inhibitors or activators or by designing new agents *de novo* via computational inspection of the three dimensional configuration and
10 electrostatic potential of an MMP-13 active site.

Accordingly, in one embodiment of the invention, the structural coordinates of Figures 4 or 5 of the present invention, or structural coordinates derived therefrom using molecular replacement or homology modeling techniques as discussed above, are used to screen a database for agents that
15 may act as potential inhibitors or activators of MMP-13 activity (or the activity of MMP-13 analogues). Specifically, the obtained structural coordinates of the present invention are read into a software package and the three dimensional structure is analyzed graphically. A number of computational software packages may be used for the analysis of structural coordinates, including, but
20 not limited to, Sybyl (Tripos Associates), QUANTA and XPLOR (Brunger, A.T., (1993) XPLOR Version 3.1 Manual, Yale University, New Haven, CT). Additional software programs check for the correctness of the coordinates with regard to features such as bond and atom types. If necessary, the three dimensional structure is modified and then energy minimized using the
25 appropriate software until all of the structural parameters are at their equilibrium/optimal values. The energy minimized structure is superimposed against the original structure to make sure there are no significant deviations between the original and the energy minimized coordinates.

The energy minimized coordinates of MMP-13 complexed with a
30 "solved" inhibitor or activator are then analyzed and the interactions between the solved ligand and MMP-13 are identified. The final MMP-13 structure is

-29-

modified by graphically removing the solved inhibitor or activator so that only MMP-13 and a few residues of the solved agent are left for analysis of the binding site cavity. QSAR and SAR analysis and/or conformational analysis may be carried out to determine how other inhibitors or activators compare to the
5 solved inhibitor or activator. The solved agent may be docked into the uncomplexed structure's binding site to be used as a template for data base searching, using software to create excluded volume and distance restrained queries for the searches. Structures qualifying as hits are then screened for activity using standard assays and other methods known in the art.

10 Further, once the specific interaction is determined between the solved inhibitor or activator, docking studies with different inhibitors or activators allow for the generation of initial models of new inhibitors or activators in complex with MMP-13. The integrity of these new models may be evaluated a number of ways, including constrained conformational analysis
15 using molecular dynamics methods (*i.e.*, where both MMP-13 and the complexed activator or inhibitor are allowed to sample different three dimensional conformational states until the most favorable state is reached or found to exist between the protein and the complexed agent). The final structure as proposed by the molecular dynamics analysis is analyzed visually to
20 make sure that the model is in accord with known experimental SAR based on measured binding affinities. Once models are obtained of the original solved agent bound to MMP-13 and computer models of other molecules bound to MMP-13, strategies are determined for designing modifications into the activators or inhibitors to improve their activity and/or enhance their selectivity.

25 Once an MMP-13 binding agent has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its selectivity and binding properties. Generally, initial substitutions are conservative, *i.e.*, the replacement group will have approximately the same size, shape, hydrophobicity and charge
30 as the

-30-

original group. Such substituted chemical compounds may then be analyzed for efficiency of fit to MMP-13 by the same computer methods described in detail above.

Alternatively, the present invention provides a method for
5 identifying a potential inhibitor or activator that is selective for one or more members of the matrix metalloproteinase family except MMP-13, comprising the steps of (i) using the three dimensional structures of MMP-13 and the desired target matrix metalloproteinase(s) as defined by the relative structural coordinates of amino acids encoding MMP-13 and the target matrix
10 metalloproteinase(s) in order to design or select such a potential inhibitor or activator, and (ii) synthesizing or obtaining said potential inhibitor or activator. In this case, the potential inhibitor or activator is designed to incorporate chemical or steric features favorable for association with an active site of the desired matrix metalloproteinase(s) and unfavorable for association with an
15 MMP-13 active site, preferably where said active site comprises the MMP-13 S1' pocket. The inhibitor or activator may be selected by screening an appropriate database, may designed *de novo* by analyzing the steric configurations and charge potentials of empty MMP-13/matrix metalloproteinase active sites in conjunction with the appropriate software programs, or may be designed using
20 characteristics of known inhibitors or activators to MMP-13 or other collagenases in order to create "hybrid" activators or inhibitors.

Various molecular analysis and rational drug design techniques are further disclosed in U.S. Patent Nos. 5,834,228, 5,939,528 and 5,865,116, as well as in PCT Application No. PCT/US98/16879, published as WO
25 99/09148, the contents of which are hereby incorporated by reference.

The present invention may be better understood by reference to the following non-limiting Examples. The following Examples are presented in order to more fully illustrate the preferred embodiments of the invention, and should in no way be construed as limiting the scope of the present invention.

Example 1

^1H , ^{15}N and ^{13}CO Assignments and Secondary Structure Determination of MMP-13 Complexed with Compound A

5

Methods and Results: The uniform ^{15}N and ^{13}C -labeled 165 amino-acid catalytic fragment of human collagenase-3 (MMP-13) was expressed in *E. coli* strain BL21(DE3) containing the plasmid pProMMP-13 according to a published method (Freije *et al.*, *J. Biol. Chem.* 1994). MMP-13 was purified as previously described (Moy *et al.*, *J. Biomol.* 1997) with minor modifications. N-terminal amino acid sequencing was performed to confirm the protein's identity while the uniform ^{15}N and ^{13}C labeling of MMP-13 was confirmed by MALDI-TOF mass spectrometry (PerSeptive Biosystems). The sulfonamide derivative of the hydroxamic acid compound, N-Hydroxy-2-[(4-methoxy-benzenesulfonyl)-pyridin-3-ylmethyl-amino]-3-methyl-benzamide, was prepared from 2-amino-3-methyl-benzoic acid methyl ester and p-methoxybenzenesulfonyl chloride followed by alkylation with 3-picolyl chloride, hydrolysis (LiOH/THF) to afford the carboxylic acid and conversion to the hydroxamic acid (oxalyl chloride/DMF/ NH_2OH). Formation of the HCl salt yielded Compound A as shown in Figure 3.

The NMR samples contained 1 mM of MMP-13 determined spectrophotometrically in a equimolar complex with Compound A in a buffer containing 10 mM deuterated Tris-Base, 100 mM NaCl, 5 mM CaCl_2 , 0.1 mM ZnCl_2 , 2 mM NaN_3 , 10 mM deuterated DTT, in either 90% H_2O / 10% D_2O or 100% D_2O at pH 6.5. All NMR spectra were recorded at 35°C on a Bruker AMX-2 600 spectrometer equipped with a triple-resonance gradient probe.

Spectra were processed using the NMRPipe software package (Delaglio *et al.*, *J. Biomol. NMR* 1995) and analyzed with PIPP (Garrett *et al.*, *J. Magn. Reson.* 1991), NMRPipe and PEAK-SORT, an in-house software package. The assignments of the ^1H , ^{15}N , ^{13}CO , and ^{13}C resonances were based on the following experiments: CBCA(CO)NH, CBCANH, C(CO)NH, HC(CO)NH,

30

-32-

HBHA(CO)NH, HNCO, HCACO, HNHA, HNCA, HCCH-COSY and HCCH-TOCSY (for reviews, see Bax *et al.*, Methods Enzymol. 1994; and Clore & Gronenborn, Methods Enzymol. 1994). The accuracy of the MMP-13 NMR assignments was further confirmed by sequential NOEs in the ^{15}N -edited NOESY-HSQC spectra.

- 5 Prior to analysis of the MMP-13 NMR structure, the structure determination of the inhibitor-free catalytic fragment of MMP-1 has been reported (Moy *et al.*, Biochemistry 1998; Moy *et al.*, J. Biomol. NMR 1997) (30 simulated annealing structures deposited with Protein Data Bank, Accession No. 1AYK; restrained minimized mean structure deposited with Protein Data Bank, 10 Accession No. 2AYK). Because the MMPs are highly autocatalytic, the NMR analysis of the inhibitor-free MMP-1 was accomplished by establishing buffer conditions where the enzyme was still active but the rate of self-cleavage of the enzyme had been diminished. This was achieved by the addition of DTT which significantly diminished self-aggregation of the enzyme and by lowering the pH 15 of the sample to 6.5, just above the pH where the enzyme was known to be inactivated because of the loss of the catalytic zinc. Under these conditions, an MMP-1 NMR sample was typically stable for 1-2 months. Unfortunately this was not the case for MMP-13, the protein rapidly degraded within a few hours which required the use of an inhibitor to assign the MMP-13 NMR resonances.
- 20 The secondary structure of the MMP-13:Compound A complex is based on characteristic NOE data involving the NH, $\text{H}\alpha$ and $\text{H}\beta$ protons from ^{15}N -edited NOESY-HSQC and ^{13}C -edited NOESY-HMQC spectra, $^3\text{JHN}\alpha$ coupling constants from HNHA, slowly exchanging NH protons and $^{13}\text{C}\alpha$ and $^{13}\text{C}\beta$ secondary chemical shifts (for reviews, see Wishart & Sykes, Methods Enzymol. 1994; and Wuthrich, NMR of Proteins and Nucleic Acids, John Wiley & Sons, 25 New York 1986). It was determined that the MMP-13 NMR structure in the complex is composed of three α -helices corresponding to residues 28-44 (α_a), 112-123 (α_b) and 153-163 (α_c) and a mixed parallel and anti-parallel β -sheet consisting of 5 strands corresponding to residues 83-86 (β_1), 95-100 (β_2), 59-66 30 (β_3), 14-20 (β_4) and 49-53 (β_5). This is essentially identical to the secondary structure observed for other MMP structures.

-33-

There were three distinct regions in the MMP-13:Compound A spectra where the resonance assignments are incomplete. These correspond to residues G70-Y73, P87-N91 and T144-H148. Residues T144-H148 correspond to part of the dynamic loop region previously seen in the MMP-1 structure (Moy
5 *et al.*, *J. Biomol. NMR* 1997). This suggests a similar dynamic profile for this region in the MMP-13 structure even in the presence of a high-affinity inhibitor ($IC_{50} = 33$ nM). Residues P87 to N91 contain a cluster of prolines which disrupt the sequential assignment process because of the missing NH. Residues G70 to Y73 correspond to a loop region in the vicinity of the structural zinc which was
10 readily assigned in the MMP-1 structure. The backbone and side-chain 1H , ^{15}N , ^{13}C , and ^{13}CO assignments are essentially complete for the remainder of the protein.

Example 2

15 High Resolution Solution Structure of the Catalytic Fragment of MMP-13 Complexed with Compound A

Materials and Methods:

Preparation of Compound A: The sulfonamide derivative of the hydroxamic acid
20 compound, Compound A, was prepared according to the procedure noted in Example 1 to yield the compound of Figure 3.

Expression of recombinant ^{15}N and ^{13}C / ^{15}N -labeled MMP-13: A 169-residue C-terminally truncated human collagenase-3 (MMP-13) was expressed in *E. coli*.
25 The coding sequence of a C-terminally truncated procollagenase was amplified by PCR from the plasmid pNot3a, that contains the entire coding sequence of MMP-13 (Frieje, *et al.*, *J. Biol. Chem.* 1994). The PCR primers contained the appropriate restriction sites for ease of cloning. The construct codes for a truncated proMMP-13 with an N-terminal methionine added and a C-terminal
30 proline at residue 169 of the native proMMP-13 sequence. The PCR amplified DNA fragment was the cloned into pET-21a (+) at the Nde I/Sal I sites ,

-34-

resulting in a recombinant plasmid designated as pProMMP-13. *E. coli* bacteria, BL21(DE3), containing the plasmid pProMMP-13, were grown in LB broth supplemented with 100 µg/ml ampicillin. An overnight culture was diluted 1:20 and grown at 37°C to an A₆₀₀ of 0.6-0.8 with vigorous shaking. Isopropyl β-D-
5 galactoside (IPTG) was added to a final concentration of 1 mM and cultures were shaken for 3 h at 37°C. The cells were harvested by centrifugation (7000 Xg for 15 min) at 4°C, washed with PBS, and frozen at -70°C until further use.

Uniform ¹⁵N and ¹³C- labeled ProMMP-13 was obtained by growing BL21(DE3) *E. coli* in defined media containing 2.0 g/l [¹³C6, 98%+]D-
10 glucose and 1.0 g/l [¹⁵N, 98%+] ammonium chloride as the sole carbon and nitrogen sources, respectively. In addition, the defined media contained M9 salts (Sambrook, *et al.*, Molecular Cloning: A Laboratory Manual, Cold Spring Harbor Laboratory Press, New York, NY 1989), trace elements, vitamins and 100 µg/ml ampicillin. Conditions for induction and growth were the same as
15 above.

Purification of recombinant ¹⁵N and ¹³C MMP-13: MMP-13 was purified according to Moy *et al.*, *J. Biomol. NMR* 1997, with modifications as follows. Frozen cell pellets were thawed on ice. Cells were resuspended by homogenization in lysis
20 buffer (0.1 M Tricine, pH 8.0, 10 mM EDTA, 2mM DTT, 0.5 mM PMSF). Cells were lysed by French Press (2X) followed by treatment with lysozyme (1 mg/ml; final) at room temperature for 30 min. The lysate was centrifuged at 45,000 x g for 30 minutes. The pellet was washed twice with 50 mM Tricine pH 7.5, 0.2 M NaCl₂, 0.5% Triton X-100, resuspended in fresh urea buffer (20 mM Tricine,
25 pH 7.5, 8 M urea, 0.2% NaN₃, 2 mM DTT) and incubated at room temperature for 1 hour. The urea solubilized protein was centrifuged at 45,000 x g for 30 min and the resultant supernatant was filtered and applied to a Hitrap-Q Sepharose (Pharmacia Biotech) anion exchange column equilibrated in 6 M urea buffer. The column was washed with urea buffer and eluted with a 0-0.25
30 M NaCl linear gradient. Fractions containing proMMP-13 were detected by SDS-PAGE, pooled and quickly diluted into 5-fold excess of renaturing buffer

-35-

(50 mM Tricine, pH 7.5, 0.4 M NaCl, 10 mM CaCl₂, 0.1 mM ZnOAc₂, 0.02% NaN₃). After 2 days of dialysis against 25 volumes of renaturing buffer (with three changes), refolded proMMP-13 was concentrated to about 4-10 mg/ml in a Millipore Biomax 5 concentrator. ProMMP-13 was activated to MMP-13CAT
5 (catalytic domain) by an overnight incubation at 37 °C in the presence of 1 mM *p*-aminophenylmercuric acetate (APMA).

The activated protein is then applied onto a Superdex-75 16/60 gel filtration column equilibrated in 2.5 mM Tris-HCl, pH 7.5, 5 mM CaCl₂, 0.4 M NaCl, 2 mM DTT, 0.02% NaN₃ and 0.05 mM ZnOAc₂. The protein is eluted
10 and fractions containing MMP-13CAT were identified by SDS-PAGE. Peak fractions were pooled and the protein was concentrated in a Millipore Biomax concentrator to about 5 mg/ml and stored at -70 °C. N-terminal amino acid sequencing was performed to confirm the protein's identity. The uniform ¹⁵N and ¹³C labeling of MMP-13-CAT was confirmed by MALDI-TOF mass
15 spectrometry (PerSeptive Biosystems).

NMR Sample Preparation: The MMP-13:Compound A NMR sample contained 1mM ¹⁵N-or ¹⁵N/¹³C-labeled MMP-13 with Compound A in a 1:1 ratio. The sample was prepared by repeated buffer exchange using 20-30ml solution
20 containing 10mM deuterated Tris-Base, 100mM NaCl, 5mM CaCl₂, 0.1mM ZnCl₂, 2mM NaN₃, 10mM deuterated DTT, and 0.2mM Compound A in either 90% H₂O/10 % D₂O or 100% D₂O. Buffer exchange was carried out on a Millipore Ultrafree-15 Centrifugal Filter Unit. Excess Compound A was removed by additional buffer exchanges where Compound A was removed from the
25 buffer.

NMR Data Collection: All spectra were recorded at 35 °C on a Bruker AMX-2 600 spectrometer using a gradient enhanced triple-resonance ¹H/¹³C/¹⁵N probe. For spectra recorded in H₂O, water suppression was achieved with the WATERGATE
30 sequence and water-flip back pulses (Piotto, *et al.*, *J. Biomol. NMR* 1992; Grzesiek and Bax, *J. Am. Chem. Soc.* 1993). Quadrature detection in the

-36-

indirectly detected dimensions were recorded with States-TPPI hypercomplex phase increment (Marion, *et al.*, J. Magn. Reson. 1989). Spectra were collected with appropriate refocusing delays to allow for 0,0 or -90,180 phase correction.

The resonance assignments and bound conformation of

- 5 Compound A in the MMP-1: Compound A complex were based on the 2D $^{12}\text{C}/^{12}\text{C}$ -filtered NOESY (Petros, *et al.*, FEBS Lett. 1992; Gemmecker, *et al.*, J. Magn. Reson. 1992), 2D $^{12}\text{C}/^{12}\text{C}$ -filtered TOCSY (Petros, *et al.*, FEBS Lett. 1992; Gemmecker, *et al.*, J. Magn. Reson. 1992) and $^{12}\text{C}/^{12}\text{C}$ -filtered COSY experiments (Ikura and Bax, J. Magn. Reson. 1992).
- 10 The MMP-13:Compound A structure is based on the following series of spectra: HNHA (Vuister and Bax, J. Am. Chem. Soc. 1993), HNHB (Archer, *et al.*, J. Magn. Reson. 1992), 3D long-range ^{13}C - ^{13}C correlation (Bax and Popchapsky, J. Magn. Reson. 1992), coupled CT-HCACO (Powers, *et al.*, J. Magn. Reson. 1991; Vuister, *et al.*, J. Am. Chem. Soc. 1992), HACAHB-COSY
- 15 (Grzesiek, *et al.*, J. Amer. Chem. Soc. 1995), 3D ^{15}N - (Mario, *et al.*, Biochemistry 1989; Zuiderweg and Fesik, Biochemistry 1989) and ^{13}C -edited NOESY (Zuiderweg, *et al.*, J. Magn. Reson. 1990; Ikura, *et al.*, J. Magn. Reson. 1990), and 3D ^{13}C -edited/ ^{12}C -filtered NOESY (Lee, *et al.*, FEBS Lett. 1994).
- 20 experiments. The ^{15}N -edited NOESY, ^{13}C -edited NOESY and 3D ^{13}C -edited/ ^{12}C -filtered NOESY experiments were collected with 100 msec, 120 msec and 110 msec mixing times, respectively. The acquisition parameters for each of the experiments used in determining the solution structure of MMP-13 complexed with Compound A were as reported previously (Moy, *et al.*, Biochemistry, 1998).
- 25 Spectra were processed using the NMRPipe software package (Delaglio, *et al.*, J. Biomol. NMR, 1995) and analyzed with PIPP (Garrett, *et al.*, J. Magn. Reson., 1991) on a Sun Sparc Workstation. When appropriate, data processing included a solvent filter, zero-padding data to a power of two, linear predicting back one data point of indirectly acquired data to obtain zero phase
- 30 corrections, linear prediction of additional points for the indirectly acquired dimensions to increase resolution. Linear prediction by the means of the mirror

-37-

image technique was used only for constant-time experiments (Zhu and Bax, J. Magn. Reson., 1992). In all cases data was processed with a skewed sine-bell apodization function and one zero-filling was used in all dimensions.

- 5 *Interproton Distance Restraints:* The NOEs assigned from 3D ^{13}C -edited/ ^{12}C -filtered NOESY and 3D ^{15}N -edited NOESY experiments were classified into strong, medium, and weak corresponding to interproton distance restraints of 1.8-2.7 Å (1.8-2.9 Å for NOEs involving NH protons), 1.8-3.3 Å (1.8-3.5 Å for NOEs involving NH protons), and 1.8-5.0 Å, respectively (Williamson, *et al.*, J. Mol. Biol., 1985; Clore, *et al.*, EMBO J., 1986). Upper distance limits for distances involving methyl protons and non-stereospecifically assigned methylene protons were corrected appropriately for center averaging (Wuthrich, *et al.*, J. Mol. Biol., 1983).
- 10
- 15 *Torsion Angle Restraints and Stereospecific Assignments.* The β -methylene stereospecific assignments and χ_1 torsion angle restraints were obtained primarily from a qualitative estimate of the magnitude of $^3J_{\alpha\beta}$ coupling constants from the HACAHB-COSY experiment (Grzesiek, *et al.*, J. Am. Chem. Soc., 1992) and $^3J_{N\beta}$ coupling constants from the HNHB experiment (Archer, *et al.*, J. Magn. Reson., 1991). Further support for the assignments was obtained from approximate distance restraints for intraresidue NOEs involving NH, C α H, and C β H protons (Powers, *et al.*, Biochemistry, 1993).
- 20

- The ϕ and ψ torsion angle restraints were obtained from $^3J_{\text{NH}\alpha}$ coupling constants measured from the relative intensity of H α crosspeaks to the NH diagonal in the HNHA experiment (Vuister and Bax, J. Am. Chem. Soc. 1993), from a qualitative estimate of the magnitude of $^3J_{\alpha\beta}$ coupling constants from the HACAHB-COSY experiment (Grzesiek, *et al.*, J. Am. Chem. Soc., 1992) and from approximate distance restraints for intraresidue and sequential NOEs involving NH, C α H, and C β H protons by means of the conformational grid search program STEREOSEARCH (Nilges, *et al.*, Biopolymers 1990), as described previously (Kraulis, *et al.*, Biochemistry 1989). $^1J_{\text{C}\alpha\text{H}\alpha}$ coupling
- 25
- 30

constants obtained from a coupled 3D CT-HCACO spectrum were used to ascertain the presence of non-glycine residues with positive ϕ backbone torsion angles (Vuister, *et al.*, *J. Am. Chem. Soc.* 1992). The presence of a $^1J_{\alpha H\alpha}$ coupling constant greater than 130 Hz allowed for a minimum ϕ restraint of -2° to -178° .

The Ile and Leu χ_2 torsion angle restraints and the stereospecific assignments for leucine methyl groups were determined from $^3J_{\alpha C\delta}$ coupling constants obtained from the relative intensity of $C\alpha$ and $C\delta$ cross peaks in a 3D long-range ^{13}C - ^{13}C NMR correlation spectrum (Bax, *et al.*, *J. Am. Chem. Soc.* 1992), in conjunction with the relative intensities of intraresidue NOEs (Powers, *et al.*, *Biochemistry* 1993). Stereospecific assignments for valine methyl groups were determined based on the relative intensity of intraresidue $NH-C\gamma H$ and $C\alpha H-C\gamma H$ NOEs as described by Zuiderweg *et al.* (1985) (Zuiderweg, *et al.*, *Biopolymers* 1985). The minimum ranges employed for the ϕ , ψ , and χ torsion angle restraints were $\pm 30^\circ$, $\pm 50^\circ$, and $\pm 20^\circ$, respectively (Kraulis, *et al.*, *Biochemistry* 1989).

Structure Calculations: The structures were calculated using the hybrid distance geometry-dynamical simulated annealing method of Nilges *et al.* (1988) (Protein Eng.) with minor modifications (Clore, *et al.*, *Biochemistry* 1990) using the program XPLOR (Brunger, *X-Plor Version 3.1 Manual*, Yale University, New Haven, CT), adapted to incorporate pseudopotentials for $^3J_{NH\alpha}$ coupling constants (Garrett, *et al.*, *J. Magn. Reson. Ser. B* 1994), secondary $^{13}C\alpha/^{13}C\beta$ chemical shift restraints (Kuszewski, *et al.*, *J. Magn. Reson. Ser. B* 1995) and a conformational database potential (Kuszewski, *et al.*, *Protein Sci.* 1996; Kuszewski, *et al.*, *J. Magn. Reson.* 1997). The target function that is minimized during restrained minimization and simulated annealing comprises only quadratic harmonic terms for covalent geometry, $^3J_{NH\alpha}$ coupling constants and secondary $^{13}C\alpha/^{13}C\beta$ chemical shift restraints, square-well quadratic potentials for the experimental distance and torsion angle restraints, and a quartic van der Waals term for non-bonded contacts. All peptide bonds were constrained to be

-39-

planar and trans. There were no hydrogen-bonding, electrostatic, or 6-12 Lennard-Jones empirical potential energy terms in the target function.

To prevent the Zn and Ca ions from being expelled during the high-temperature simulated annealing stages of the refinement protocol, a minimal number of distance restraints between the His sidechain and Zn and between backbone atoms and C α were included in the XPLOR distance restraint file based on the observed coordination in the X-ray structures (Lovejoy, *et al.*, Science 1994; Lovejoy, *et al.*, Biochemistry 1994; Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994; Borkakoti, *et al.*, Nat. Struct. Biol. 1994).

The starting MMP-13:Compound A complex structure for the simulated-annealing protocol was obtained by manually docking Compound A into a homology model for MMP-13. The initial orientation of Compound A in the MMP-13 active site was based on the previously reported MMP-1:CGS-27023A structure (Moy, *et al.*, Biochemistry 1999).

Homology modeling methods were utilized to generate a three dimensional model of MMP-13. The linear amino acid sequence corresponding to the catalytic domain of MMP-13 was aligned (SYBYL) with the catalytic domains of MMP-1, MMP-7 and MMP-8 based on the availability of their x-ray crystallographic structures (Bode, *et al.*, EMBO J 1994; Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994; Betz, *et al.*, Eur. J. Biochem. 1997; Lovejoy, *et al.*, Nat. Struct. Biol. 1999; Borkakoti, *et al.*, Nat. Struct. Biol. 1994; Browner, *et al.*, Biochemistry 1995). The alignments of MMP-13 with MMP-1 and MMP-8 demonstrated the highest homology where the computed identities are 58.9% and 61.4%, respectively (Figure 2).

The X-ray structure of MMP-8 was selected to be used as the template for homology modeling the structure of MMP-13. This decision was based mainly on the sequence alignment shown in Figure 2B where no insertions (labeled “###”) are found in the critical specificity loop (Labeled Underlined and Boldface). In Figure 2A, the region labeled “##” in the specificity loop shows that there is an “insertion” of 2 additional amino acid residues compared to the sequence length of MMP-1. Based on our analysis of

-40-

the alignments, MMP-8 would allow for a more accurate modeling of the inhibitor binding pockets since no predictions have to be made within this loop region.

COMPOSER (SYBYL) was used to construct the initial homology
5 model of MMP-13. The only insertion was a serine (labeled '**' in Figure 2B) at position 32 of MMP-13. The insertion of S32 occurs within a coiled region which is at the entrance of a long alpha helix and about 17 angstroms from the S' specificity loop. The model of MMP-13 was then energy minimized utilizing a set of nested refinement procedures (Chen, *et al.*, J. Biomol. Struct. Dyn. 1995),
10 but where the protein backbone heavy atoms were constrained as close as possible to their original positions.

The MMP-13:Compound A model was then subjected to a 1000 steps of CHARMM minimization with the 5 intramolecular NOE restraints and the 47 distance restraints observed between MMP-13 and Compound A where
15 the coordinates for MMP-13 were kept fixed. This approach approximated the positioning of Compound A in the active site of MMP-13 without distorting the MMP-13 structure. The final structure was exported as a PDB file and used as the starting point for XPLOR simulated annealing protocol where all the residues in the structure were free to move. Since the initial stage of the
20 simulated annealing protocol corresponds to high-temperature dynamics (1500 K) with a relatively weak XPLOR NOE force constant (Ries and Petrides, Biol. Chem. Hoppe-Seyler 1995), the initial MMP-13:Compound A structure does not bias the structure determination process since the structure is effectively free to explore the available conformational space. Additionally, each iteration of the
25 simulated annealing process begins with a random trajectory for the molecular dynamics. The fact that these trajectories differ by upwards of 10 Å assures a distinct exploration of conformational space for the ensemble of MMP-13:Compound A structures determined from the simulated annealing protocol.

Results and Discussion

Compound A Resonance Assignments and Bound Conformation: The primary structure of Compound A along with the proton naming convention is shown in Figure 3. The NMR assignments for Compound A in the MMP-13 complex followed established protocols using 2D ^{13}C -filtering experiments (Petros, *et al.*, FEBS Lett. 1992; Gemmecker, *et al.*, J. Magn. Reson. 1992; Ikura and Bax, J. Am. Chem. Soc. 1992) since the NMR sample was composed of $^{13}\text{C}/^{15}\text{N}$ labeled MMP-13 and unlabeled Compound A. Thus, traditional 2D-NOESY, COSY and TOCSY spectra of Compound A in the presence of MMP-13 yielded straight-forward assignments for Compound A along with assignments for free Compound A (data not shown). The only notable difference in the assignments for free and bound Compound A is the observation of two distinct resonances for 2HB1/2 in the complex (4.91 ppm; 4.67 ppm). The missing resonance in the free Compound A may simply be obscured by water. Also, an observation that the protons on the p-methoxyphenyl ring are degenerate suggests rapid ring flips when complexed to MMP-13. This was also seen with CGS-27023A complexed with both MMP-1 and stromelysin (Gonnella, *et al.*, Bioorg. Med. Chem. 1997; Moy, *et al.*, Biochemistry 1998; Moy, *et al.*, Biochemistry 1999).

Compound A does not adopt a preferred conformation in the absence of MMP-13 as evident by the lack of structural NOEs. Only a minimal number of intramolecular NOEs were observed for Compound A in the MMP-13 complex which were relevant to the bound conformation of Compound A (data not shown). The minimal number of structural NOEs is a result of the Compound A conformation, structure and chemical shift degeneracy. A number of the observed NOEs correspond to a sequential interaction which have no effect on the overall conformation of the inhibitor and were not used in the refinement of Compound A or the complex. The structural intramolecular NOEs observed are primarily between 1HH* and the pyridine ring and between 2HB1/2 and both the p-methoxyphenyl and aryl ring. These NOEs are consistent with the "splayed" conformation previously observed for CGS-27023A bound to both MMP-1 and stromelysin, but the bound conformation of

-42-

Compound A is predominately determined from the intermolecular NOEs between Compound A and MMP-13 (Table 1).

Structure Determination: The NMR structure determination methodology is an iterative procedure where the current state of the structure is used to analyze the ambiguous NOE data. In essence, the structure is used as a distance filter to sort through the ambiguous NOE list where the first structure is determined from unambiguous data. For the refinement of MMP-13, the initial structure was a homology model based on the MMP-8 X-ray structure. This was justified by the overall similarity in previously reported MMP structures and from the secondary structure assignments by NMR for MMP-13. The regular secondary structure elements of MMP-13 were identified from a qualitative analysis of sequential and inter-strand NOEs, NH exchange rates, $^3\text{JHN}\alpha$ coupling constants (Clare, *et al.*, Crit. Rev. Biochem. Mol. Biol. 1989) and the $^{13}\text{C}\alpha$ and $^{13}\text{C}\beta$ secondary chemical shifts (Spera and Bax, J. Am. Chem. Soc. 1991). The deduced secondary structure is essentially identical to the inhibitor-free MMP-1 NMR structures previously reported.

The final 30 simulated annealing structures calculated for residues 7-164 were based on 3279 experimental NMR restraints, consisting of 2561 approximate interproton distance restraints, 51 distance restraints between MMP-13 and Compound A, 88 distance restraints for 44 backbone hydrogen bonds, 391 torsion angle restraints, 103 $^3\text{J}_{\text{NH}\alpha}$ restraints 123 $\text{C}\alpha$ restraints and 108 $\text{C}\beta$ restraints. Stereospecific assignments were obtained for 81 of the 100 residues with β -methylene protons, for the methyl groups of 5 of the 6 Val residues, and for the methyl groups of 12 of the 13 Leu residues. In addition, 12 out of the 12 Phe residues and 7 out of the 8 Tyr residues were well defined making it possible to assign NOE restraints to only one of the pair of $\text{C}\delta\text{H}$ and $\text{C}\epsilon\text{H}$ protons and to assign a χ^2 torsion angle restraint. Similarly, χ^2 torsion angle restraints were assigned for the three Trp residues. The atomic rms distribution of the 30 simulated annealing structures about the mean coordinate positions for residues 7-164 is $0.43 \pm 0.06 \text{ \AA}$ for the backbone atoms, $0.81 \pm$

-43-

0.09 Å for all atoms, and 0.47 ± 0.04 Å for all atoms excluding disordered surface side chains. The mean standard deviation for the ϕ and ψ backbone torsion angles of residues 7-164 are $6.2 \pm 11.3^\circ$ and $7.1 \pm 11.8^\circ$, respectively. The high quality of the MMP-13 NMR structure is also evident by the results of PROCHECK analysis and by a calculated, large negative value for the Lennard-Jones-van der Waals energy (-695 ± 11 kcal mol⁻¹). For the PROCHECK statistics, an overall G-factor of 0.16 ± 0.16 , a hydrogen bond energy of 0.82 ± 0.05 and only 7.8 ± 1.0 bad contacts per 100 residues are consistent with a good quality structure comparable to ~ 1 Å X-ray structure.

The high quality of the MMP-13 NMR structure is also evident by the very small deviations from idealized covalent geometry, by the absence of interproton distance and torsion angle violations greater than 0.1 Å and 1° , respectively and by the fact that most of the backbone torsion angles for non-glycine residues lie within expected regions of the Ramachandran plot (not shown). 91.5% of the residues lie within the most favored region of the Ramachandran ϕ , ψ plot and 7.8% in the additionally allowed regions. ¹JCαHα coupling constants from the coupled CT-HCACO experiment indicated that all non-glycine residues have negative ϕ torsion angles.

The quality of the NMR data to properly define the complex is also supported by the well-defined coordinates for Compound A and the active site residues, where the atomic rms distribution is 0.47 ± 0.08 Å and 0.18 ± 0.03 Å for the heavy atoms of Compound A and MMP-13 backbone atoms, respectively.

Description of the MMP-13:Compound A Structure: The overall fold of MMP-13 is essentially identical to previously reported MMP structures (Bode, *et al.*, EMBO J. 1994; Gooley, *et al.*, Nat. Struct. Biol. 1994; Lovejoy, *et al.*, Science 1994; Lovejoy, *et al.*, Ann. N. Y. Acad. Sci. 1994; Lovejoy, *et al.*, Biochemistry 1994; Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994; Stams, *et al.*, Nat. Struct. Biol. 1994; Becker, *et al.*, Protein Sci. 1995; Gonnella, *et al.*, Proc. Natl. Acad. Sci. U. S. A. 1995; Van Doren, *et al.*, Protein Sci. 1995; Botos, *et al.*, Proc. Natl. Acad. Sci. USA 1996; Broutin, *et al.*, Acta Crystallogr., Sect. D: Biol. Crystallogr.

-44-

1996; Gooley, *et al.*, J. Biomol. NMR 1996; Betz, *et al.*, Eur. J. Biochem. 1997; Gonnella, *et al.*, Bioorg. Med. Chem. 1997; Moy, *et al.*, Biochemistry 1998 and Moy, *et al.*, Biochemistry 1999). The MMP-13 NMR structure is composed of three α -helices corresponding to residues 28-44 (α_A), 112-123 (α_B) and 153-163 (α_C) and a mixed parallel and anti-parallel β -sheet consisting of 5 strands corresponding to residues 83-86 (β_1), 95-100 (β_2), 59-66 (β_3), 14-20 (β_4) and 49-53 (β_5). The active site of MMP-13 is bordered by β -strand IV, the Ca^{+2} binding loop, helix B and a random coil region from residues P139-Y141. The catalytic zinc is chelated by H119, H123, and H129 while the structural zinc is chelated by H69, H84 and H97. The calcium ion is chelated in a loop region consisting of residues D75 to G79. An interesting feature of the MMP active-site structure is an apparent kink in the backbone that occurs between the Ca^{+2} binding loop and β -strand IV. In the case of MMP-13, this results in the NHs of both L82 and A83 facing toward the active site of the enzyme. An important feature of substrate and inhibitor binding to the MMPs are hydrogen bonding interactions with β -strand IV which is facilitated by this unusual kink conformation (Lovejoy, *et al.*, Science 1994; Lovejoy, *et al.*, Biochemistry 1994; Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994; and Borkakoti, *et al.*, Nat. Struct. Biol. 1994).

20 The interaction of Compound A in the active site of MMP-13 was determined by 5 intramolecular NOEs for Compound A and by a total of 47 intermolecular distance restraints between MMP-13 and Compound A. The key MMP-13 residues involved in the interaction with the inhibitor correspond to three distinct MMP-13 regions: residues L81, L82 and A83 from β -strand IV; residues L115, V116, and H119 from α -helix II; and L136, I140 and Y141 from the active site loop which comprise the S1' and S2' pockets of MMP-13. A unique feature of the MMP-13 structure is the large S1' pocket which nearly reaches the surface of the protein.

30 Compound A binds to the right-side of the catalytic Zn where the p-methoxyphenyl of Compound A sits in the S1' pocket of the MMP-13 active site. This positioning is evident from the observed NOEs from 3HH*, 3HE1/2

-45-

and 3HD1/2 to L115, V116, H119, L136, and Y141. The aryl group primarily interacts with the side-chain of L81 as evident by the strong NOEs between 1HH*, 1HE2 and 1HZ and the L81 spin-system. Finally, the pyridine ring is essentially solvent exposed but interacts with the side-chain of I140. These interactions position Compound A such that the hydroxamic acid moiety of Compound A chelates to the “right” of the catalytic zinc and the sulfonyl oxygens are in hydrogen-bonding distance to the backbone NH of L82.

It is interesting to note that the active site loop is highly dynamic in both the inhibitor-free and CGS-27023A structures based on S² order-parameters (Moy, *et al.*, *J. Biomol. NMR* 1997). This region in the MMP-13:Compound A structure appears to be significantly less mobile by the observation that most of the residues in this loop region were easily observable in the ¹H-¹⁵N HSQC spectra and readily assigned. One possible explanation for this difference is the hydrophobic interaction between the pyridine ring of Compound A and the side-chain for Ile-140. In MMP-1, I140 is replaced by a serine which essentially eliminates this beneficial interaction.

Another unique feature of the MMP-13 NMR structure is the apparent dynamic nature of residues H69 to Y73. These residues are completely disordered due to the lack of any assignment information and the resulting absence of any constraint information presumably a result of the flexible nature of these residues. Residues H69 to Y73 occur between the Ca⁺² binding loop and the structural zinc where the corresponding region in the previously solved MMP-1 NMR structures is well defined. There is no apparent explanation for this change in mobility between the two NMR structures but it may contribute to the observed difference in the physical behavior of MMP-1 and MMP-13. Under identical conditions, inhibitor-free MMP-1 is stable for upwards of two months whereas inhibitor-free MMP-13 degrades immediately.

Comparison of the MMP-13:Compound A and MMP-1:CGS-27023A Structures:

The high-resolution NMR structure for the MMP-13:Compound A complex was effectively and efficiently determined by using a homology model based on the

-46-

MMP-1 NMR structure as an initial structure to analyze ambiguous NOESY data. This result is evident of the high structural and sequence similarity between members of the MMP family and consistent with the previously observed best-fit superposition of the backbone atoms for MMP-1, stromelysin, matrilysin and
5 neutrophil collagenase (Moy, *et al.*, Biochemistry 1998; Moy, *et al.*, Biochemistry 1999).

The strong similarity between the various MMP structures creates an initial difficulty in designing specific MMP inhibitors. This is exemplified by the high sequence similarity among the MMPs in the active site. Comparison of
10 the sequence similarity between MMP-13 and MMP-1 illustrates this difficulty. There are only a few significant residue differences between the two enzymes where these modifications results in a significant change in the local environment of the active site. The R114 to V115 modification results in a conversion from a hydrophilic to a hydrophobic environment at the base of the
15 S1' pocket between MMP-1 and MMP-13, respectively. Similarly, the N80 to L81 substitution places a bulkier hydrophobic residue in the S2' pocket for MMP-13 compared to a more hydrophilic environment for MMP-1. Similarly in the active loop region, I140 a bulky hydrophobic residue in MMP-13 replaces the smaller hydrophilic S139 residue in MMP-1. Clearly, it is feasible to
20 incorporate substituents into a small molecule to take advantage of these spatial distinct environmental changes between MMP-1 and MMP-13. Nevertheless, when these sequence and environmental differences are averaged across the MMP family it becomes less discriminating and extremely difficult to design an inhibitor to a specific MMP subtype based strictly on the small sequence
25 differences.

Conversely, the most distinct structural difference between the MMPs and readily amenable to incorporating specificity in drug design is the relative size and shape of the S1' pocket. This is clearly evident by comparison of the defined S1' pockets for MMP-13 and MMP-1. The large difference in size
30 in the S1' pockets between the MMP-13 and MMP-1 NMR structures is striking. The S1' pocket for MMP-13 nearly reaches the outer surface of the protein and

-47-

is greater than twice the size of MMP-1. The additional size of the MMP-13 S1' pocket relative to MMP-1 is best illustrated by the filling capacity of the two inhibitors. In the MMP-1:CGS-27023A NMR structure, the p-methoxyphenyl effectively fills the available S1' pocket for MMP-1. Conversely, in the MMP-13:Compound A complex the p-methoxyphenyl only partially fills the available space within the MMP-13 S1' pocket. The size of the MMP-13 pocket is actually similar in size to stromelysin where the design of stromelysin inhibitors has taken advantage of this deeper S1' pocket by using a biphenyl substituent in another series instead of the p-methoxyphenyl in Compound A to bind into the S1' pocket (Hajduk, *et al.*, J. Am. Chem. Soc. 1997; Olejniczak, *et al.*, J. Am. Chem. Soc. 1997). Thus, the NMR structures for MMP-13 and MMP-1 suggest that a ready approach to designing specificity between these MMPs is to take advantage of the significantly different sized S1' pockets. The high mobility of the MMP-1 active site presents a potential caveat to this analysis of the static images of the MMP-1 and MMP-13 structures. It is probable that the MMP-1 active site is capable of accommodating a S1' substituent larger than implied from its current structure due to its increased mobility in both free and inhibited structures.

Examination of the binding mode of Compound A in the MMP-13:Compound A complex suggests a conformation generally similar to CGS-27023A in the MMP-1:CGS-27023A NMR structure previously reported (30 simulated annealing structures deposited with Protein Data Bank, Accession No. 4AYK; restrained minimized mean structure deposited with Protein Data Bank, Accession No. 3AYK). Compound A and CGS-27023A are structurally very similar with the only difference being the nature of the substituent binding in the S2' pocket where an aryl group in Compound A replaces the isopropyl group in CGS-27023A. The strong resemblance between the binding mode of Compound A and CGS-27023A is apparent from the nearly identical intermolecular NOE patterns observed between the inhibitors and the proteins. The key MMP-13 residues involved in the interaction with Compound A correspond to L81, L82 and A83 from β -strand IV; residues L115, V116, and

-48-

H119 from α -helix II; and L136, I140 and Y141 from the active site loop. Similarly, the MMP-1 residues involved in the interaction with CGS-27023A correspond to residues N80, L81, A82 and H83 from β -strand IV; residues R114, V115, H118 and E119 from α -helix II; and L135, P138, Y137, S139 and
5 Y140 from the dynamic flexible loop.

As stated previously, there are three distinct residue changes between MMP-13 and MMP-1 in the active site. The R114 to L115 change between MMP-1 and MMP-13, respectively, has a significant impact on the environment at the base of the S1' pocket but since Compound A only partially
10 fills the MMP-13 S1' pocket this change should not effect the binding conformation of Compound A relative to CGS-27023A. Conversely, the N80 to L81 substitution directly interacts with the inhibitors in the S2' pocket and may result in an effective change in the binding mode of the inhibitors. To complicate the analysis, the only change in the inhibitors are the substituents
15 that bind the S2' pocket. For the MMP-1:CGS-27023A complex, the isopropyl group interacts with both the sidechains of N80 and H83 where the aryl group from Compound A only interacts with L81 in MMP-13. Additionally, CGS-27023A is in hydrogen-bonding distance to both L81 and A82, whereas Compound A appears to form a bifurcated hydrogen bond with L82. This
20 analysis suggests that CGS-27023A binds closer to β -strand IV since the S2' pocket is more accessible in MMP-1 due to the absence of the bulky L81 side-chain and the presence of the aryl group in Compound A. A direct comparison of the bound conformations suggest only a subtle difference in the relative orientation of the inhibitors. The S139 to I140 difference between MMP-1 and
25 MMP-13, respectively, appears to be related to a mobility change as opposed to a structural change. In the MMP-1:CGS-27023A structure the pyridine ring position is essentially undefined and solvent exposed this compares to the MMP-13:Compound A structure where the pyridine ring binds with the side-chain of I140. Clearly, Ile is a bulkier more hydrophobic group relative to Ser which
30 would provide a beneficial hydrophobic interactions with the pyridine ring. The more interesting observation is the apparent decrease in mobility for the active

-49-

loop in the MMP-13 structure which may be related the pyridine ring I140 interaction. This appears to be consistent with previously inhibited MMP X-ray structures (Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994) where the inhibitor may extend the formation of a β -sheet between b-strand IV and the active loop region which results in low B-factors in the X-ray structure. This may suggest that the mobility of the active loop region is easily removed with any positive interaction with the inhibitor.

There are apparently some interesting differences between the mode of binding for the two inhibitors in the MMP-13:Compound A and MMP-1:CGS-27023A NMR structures. The more striking observation is the overall similarity between the two structures. Despite some significant sequence differences and a large difference in the size and shape of the S1' pocket either inhibitor structure would accurately predict the other structure. This observation seems to indicate that the major contributing factors to inhibitors binding the MMPs is the fit in the S1' pocket and the binding of the hydroxamic acid to the catalytic zinc. The interaction in the S2' pocket appears to have a more subtle impact on inhibitor binding and selectivity since both Compound A and CGS-27023A are low nanomolar inhibitors of MMP-13 and MMP-1, respectively. Therefore, the high-resolution solution structure of the MMP-13:Compound A in conjunction with the previously reported MMP-1 NMR structures suggest that taking advantage of the significant differences in the size and shape of the S1' pocket is a reasonable approach for developing specific MMP inhibitors.

The studies described herein present the high-resolution solution structure of MMP-13 complexed with a sulfonamide derivative of a hydroxamic acid compound (Compound A). The overall fold of MMP-13 is similar to previously reported MMPs structures. The major difference is the large S1' pocket which nearly reaches the surface of the protein. The structure was based on a total of 3279 constraints including 47 distance restraints between MMP-13 and Compound A from X-filtered NOESY experiments. The inhibitor was found to bind to the "right" side of the catalytic Zn such that the p-methoxyphenyl ring

-50-

- sits in the S1' pocket, the aryl moiety interacts with L81 of β IV, the pyridine ring interacts with I140 of the active site loop, hydrogen bond interactions exist between the sulfonamide oxygens with residue L82 and the hydroxamic acid chelates the catalytic Zn. This inhibitor binds MMP-13 similarly to the MMP-1:
- 5 CGS-27023A complex suggesting that appropriately filling the S1' pocket may play a key role in developing selective MMP inhibitors.

Table 1. Observed NOEs Between Compound A and MMP-13

| Compound A | MMP-13 | NOE Class | Compound A | MMP-1 | NOE Class |
|------------|--------------------|-----------|------------|-------------------|-----------|
| 1HH* | L81 Hy | W | 3HH* | Y141 H α | M |
| 1HH* | L81 H δ 1# | W | 3HH* | Y141 H β 1 | W |
| 1HH* | L81 H δ 2# | M | 3HH* | Y141 H β 2 | W |
| 1HH* | L81 H α | S | 3HH* | Y141 H δ 2 | W |
| 1HE2 | L81 H δ 1# | W | 3HE2 | L82 H δ 1# | W |
| 1HE2 | L81 H δ 2# | M | 3HE1 | A83 H β # | W |
| 1HZ | L81 H δ 1# | W | 3HE1 | H116 H α | W |
| 1HZ | L81 H δ 2# | M | 3HE1 | H116 Hy1# | M |
| 2HZ | I140 Hy2# | W | 3HE2 | H116 Hy2# | W |
| 2HE1 | I140 H δ 1# | W | 3HE2 | I140 Hy2# | W |
| 3HH* | L82 H δ 1# | W | 3HE2 | Y141 H α | W |
| 3HH* | L115 H β # | W | 3HE2 | Y141 H β 1 | W |
| 3HH* | L115 Hy | W | 3HE2 | Y141 H β 2 | W |
| 3HH* | L115 H δ 1# | W | 3HD2 | L82 H δ 1# | W |
| 3HH* | L115 H δ 2# | W | 3HD1 | A83 H β # | W |
| 3HH* | V116 H α | W | 3HD1 | V116 Hy1# | W |
| 3HH* | V116 Hy1# | W | 3HD2 | V116 Hy2# | W |
| 3HH* | V116 Hy2# | M | 3HD2 | I140 H α | W |
| 3HH* | H119 H α | W | 3HD2 | I140 Hy2# | W |
| 3HH* | H119 H δ 2 | W | 3HD2 | Y141 H α | W |
| 3HH* | H119 H β 1 | W | 3HD2 | Y141 H β 1 | W |
| 3HH* | H119 H β 2 | W | 3HD2 | Y141 H β 2 | W |
| 3HH* | L136 H δ 1# | W | 3HD2 | Y141 HN | W |
| 3HH* | L136 H δ 2# | W | | | |

Example 3

Structure Based Design of a Novel, Potent, and Selective Inhibitor for MMP-13

The matrix metalloproteinases (MMPs) comprise a family of zinc
5 containing enzymes that cleave a broad range of substrates including collagens,
fibronectin and gelatins where the substrate preference varies for individual
MMPs. The design of MMP inhibitors has been initially based upon imitation of
the binding interaction of natural protein substrates to MMPs where structural
information of MMPs complexed with peptide substrates has been determined
10 by x-ray crystallography and NMR spectroscopy. This structural information has
provided a general description of the MMPs active site.

The active site for the MMPs is composed of a catalytic zinc
chelated by three histidines where three substrate binding pockets are located to
both the right (S1', S2', S3') and left (S1, S2, S3) of the catalytic zinc. The
15 substrate binding pockets were identified by the interactions of side chains from
the peptide substrate with the MMPs. The primary effort in MMP inhibitor
design has focused on compounds that chelate the catalytic zinc while primarily
binding in the S1' and S2' pockets. This has evolved from the observation that
the structural characteristics of the S1' pocket (size, shape, amino acid
20 composition) incurs the greatest variability between the individual MMPs and
this provides an obvious approach in designing selective and specific MMP
inhibitors. Nevertheless, there has also been success in utilizing the binding
pockets to the left of the catalytic zinc in addition to or in combination with the
right handed binding pockets in the design of inhibitors.

25 The underlying challenge in designing MMP inhibitors is the
reasonably high sequence and structural homology observed between the
individual members of the MMP family making it intrinsically difficult to design
an inhibitor that will function against a single MMP in the absence of structural
information. The problem with a non-specific MMP inhibitor as a drug is the
30 high likelihood of serious side-effects because of the large number of enzymes in
the MMP family and their corresponding diversity in targets and function.

-53-

Accordingly, the detailed structural information provided herein is a critical component of an inhibitor design program targeting a particular MMP enzyme.

Materials and Methods:

- 5 *Synthesis of Compound D and Compound E:* The sulfonamide derived from 2-amino-3,5-dimethyl-benzoic acid methyl ester and p-methoxybenzenesulfonyl chloride was N-alkylated with benzyl bromide and the ester group of the resulting intermediate was hydrolyzed (LiOH/THF) to afford the carboxylic acid. The corresponding hydroxamic acid was formed by preparation of the
10 acid chloride (oxalyl chloride/DMF) followed by reaction with hydroxylamine. Compound E was synthesized by reaction of 2-amino-3,5-dimethyl-benzoic acid methyl ester and p-fluorobenzenesulfonyl chloride followed by N-alkylation with benzyl bromide. Hydrolysis of the methyl ester (LiOH/THF) followed by displacement of fluorine with the alkoxide of benzofuran-2-carboxylic acid (2-
15 hydroxy-ethyl)-amide gave, after conversion to the hydroxamic acid and formation of the HCl salt as described above, Compound E.

- NMR Sample Preparation:* Uniformly (>95%) ^{15}N - and $^{15}\text{N}/^{13}\text{C}$ -labeled human recombinant MMP-13 was expressed in *E. coli* and purified as described
20 previously. 1mM $^{13}\text{C}/^{15}\text{N}$ - and ^{15}N - MMP-13 NMR samples were prepared by concentration and buffer exchange using Millipore Ultrafree -10 centrifugal filters into a buffer containing 10mM deuterated Tris-base, 100mM NaCl, 5mM CaCl_2 , 0.1 mM ZnCl_2 , 2 mM NaN_3 , 10mM deuterated DTT in 90% $\text{H}_2\text{O}/10\% \text{D}_2\text{O}$ or 100% D_2O . The 10:1 Compound B:MMP-13 samples were prepared by
25 addition of Compound B into either a 1mM $^{13}\text{C}/^{15}\text{N}$ - or ^{15}N -MMP-13 sample followed by pH readjustment. The sample to explore the potential of competitive inhibition between Compound B and Compound A was prepared by first adding 1mM of Compound A to a 1 mM ^{15}N - MMP-13 sample followed by the addition of 10mM Compound B. The initial MMP-13:Compound A sample
30 was made by buffer exchange of ^{15}N - MMP-13 into the buffer containing 0.1 mM Compound A followed by additional buffer exchanges to remove excess

Compound A. Finally, 10mM of Compound B was added to the 1mM ^{15}N - MMP-13:Compound A sample followed by pH readjustment.

NMR Data Collection: All spectra were recorded at 35°C on a Bruker AMX-2 600 spectrometer using a gradient enhanced triple-resonance $^1\text{H}/^{13}\text{C}/^{15}\text{N}$ probe. For spectra recorded in H_2O , water suppression was achieved with the WATERGATE sequence and water-flip back pulses (Piotto, *et al.*, J. Biomol. NMR 1992; Grzesiek and Bax, J. Am. Chem. Soc. 1993). Quadrature detection in the indirectly detected dimensions were recorded with States-TPPI hypercomplex phase increment (Marion, *et al.*, J. Magn. Reson. 1989). Spectra were collected with appropriate refocusing delays to allow for 0,0 or -90,180 phase correction.

The resonance assignments and bound conformation of Compound A in the MMP-1: Compound A complex were based on the 2D $^{12}\text{C}/^{12}\text{C}$ -filtered NOESY (Petros, *et al.*, FEBS Lett. 1992; Gemmecker, *et al.*, J. Magn. Reson. 1992), 2D $^{12}\text{C}/^{12}\text{C}$ -filtered TOCSY (Petros, *et al.*, FEBS Lett. 1992; Gemmecker, *et al.*, J. Magn. Reson. 1992) and $^{12}\text{C}/^{12}\text{C}$ -filtered COSY experiments (Ikura and Bax, J. Am. Chem. Soc. 1992).

The assignments of the ^1H , ^{15}N , and ^{13}C resonances of MMP-13 in the MMP-13:Compound B complex were based on the previous assignments for the MMP-13:Compound A complex in combination with a minimal set of experiments: 2D ^1H - ^{15}N HSQC, 3D ^{15}N - edited NOESY (Marion, *et al.* Biochemistry 1989; Zuiderweg and Fesik, Biochemistry 1989), CBCA(CO)NH (Grzesiek and Bax, J. Am. Chem. Soc. 1992), C(CO)NH (Grzesiek, *et al.*, J. Magn. Reson., Ser. B 1993), HNHA (Vuister and Bax, J. Am. Chem. Soc. 1993) and HNCA (Kay, *et al.*, J. Magn. Reson. 1990). The acquisition parameters for each of the experiments used in determining the solution structure of the MMP-13:Compound B complex were as reported previously (Moy, *et al.*, Biochemistry 1996).

The MMP-13:Compound B structure is based on observed NOEs from the 3D ^{15}N -edited NOESY (Marion, *et al.* Biochemistry 1989; Zuiderweg and Fesik, Biochemistry 1989) and 3D ^{13}C -edited/ ^{12}C -filtered NOESY (Vuister

and Bax, *J. Am. Chem. Soc.* 1993; Lee, *et al.*, *FEBS Lett.* 1994). The 3D ¹⁵N-edited NOESY and 3D ¹³C-edited/¹²C-filtered NOESY experiments were collected with 100 msec and 110 msec mixing times, respectively.

5 *Molecular Analysis and Design:* The minimized models of Compound B and Compound D complexed to MMP-13 were prepared as previously described (Chen, *et al.*, *J. Biomol. Struct. Dyn.* 1995; Chen, *et al.*, *Biochemistry* (in press) 1998). Using molecular dynamics methods (Sybyl v6.4 from Tripos Inc), protein regions within 5 Å from Compound B were sampled along with the inhibitor,
10 whereas everything else remained rigid during the simulations. Upon energy convergence, the last 50 frames from the final 100 picoseconds run was averaged and this averaged structure underwent a final minimization. The final protein-Compound B model appeared to have optimized possible polar and van der waals interactions. The identical procedure was applied to the complex of
15 MMP-13 and Compound D. Since the two complexes used identical MMP-13 structures, the proteins were overlapped to depict the positions of the two inhibitors within the active site. Graphics analysis of the inhibitors showed that the methylene carbon of Compound B containing the 2HB1/2 protons (Figure 6) overlapped identically with the methoxy carbon from Compound D. This
20 analysis indicated the optimal or minimal linkage length of connecting the benzofuran moiety to the methoxy region of Compound D. The final design scheme is shown in Figure 8A for the hybrid inhibitor. The homology model of MMP-9 was constructed using the COMPOSER program (Tripos INC, Sybyl v.6.4)

25

High-throughput Screening Analysis: Compound B was identified as an initial lead from the analysis of the MMP-13 high-throughput screen (HTS). A total of 58079 compounds were screened for their ability to inhibit MMP-13 enzymatic activity where 385 compounds were shown to have ≥ 40% inhibition at 10
30 µg/ml dosage. Compound B was shown to exhibit weak inhibition of MMP-13 (89% at the 10 µg/ml), but more intriguing was the observation of a complete

lack of activity against other MMPs (MMP-1, MMP-9 and TACE). The primary structure of Compound B along with the proton naming convention is shown in Figure 6.

The resulting HTS hits were further examined by cluster analysis.

5 The hits were clustered based on structural similarities where the properties of these compounds were compared against the properties of the set of orally available drugs. The properties used to profile the HTS hits consists of: total number of non-hydrogen atoms, number of heteroatoms, number of hydrogen-bond donors and acceptors, calculated logP and molecular weight. This profile
10 analysis provides an initial means to predict the likelihood that an HTS hit may have drug-like characteristics such as bioavailability and in-vivo stability. The profile of Compound B indicates that the compound has properties similar to orally available drugs suggesting that it would be an ideal candidate for optimization of its enzyme potency and selectivity.

15 A common feature of known MMP inhibitor structures is the presence of a Zn-chelator that plays a fundamental role in its activity. In most cases Zn chelation occurs from the presence of a hydroxamic acid in the structure of the small molecule. As apparent from the structure of Compound B, the compound does not contain an obvious substituent that would chelate Zn.
20 Thus, the unique structure of Compound B suggested a potential novel mechanism for inhibition of MMP-13 further strengthening the choice of Compound B as an initial lead candidate. Therefore, the identification of Compound B as a candidate to optimize its activity and selectivity was based on three unique observations: its intrinsic MMP-13 selectivity, its structural profile
25 similar to known bioavailable drugs and finally its apparent novel structure.

NMR Structure of the MMP-13 - Compound B Complex: The NMR binding studies provided critical information pertaining to the mechanism of Compound B inhibition of MMP-13 and the method for designing increase potency. The
30 major question presented when Compound B was identified from HTS was its unknown MMP-13 binding site and its method for inducing MMP-13 inhibition.

Previous work on the NMR structure of MMP-13 complexed with Compound A and MMP-1 complexed with CGS-27023A provided the framework and methodology to analysis Compound B bound to MMP-13 (Moy, *et al.*, Biochemistry Submitted 1999; Moy, *et al.*, Biochemistry 1999).

- 5 The Compound B MMP-13 binding site was initially identified from chemical shift perturbation in the ^1H - ^{15}N HSQC spectra. The observed perturbations were mapped onto a GRASP surface (not shown). It is apparent that the major effect of Compound B on the chemical shifts of MMP-13 occurs in the proximity of the S1' pocket suggesting that Compound B sits in this pocket.
- 10 From the NMR and X-ray structures of MMP-13, it was determined that the S1' pocket for MMP-13 is very deep and linear in shape while nearly reaching the surface of the protein. In fact, a number of residues at the surface of MMP-13 near the base of the S1' pocket show significant chemical shift perturbation in the presence of Compound B. Since Compound B is a linear molecule, docking
- 15 studies would place the inhibitor stretched throughout the linear S1' pocket of MMP-13. The only question remaining was whether to place the morpholine or the benzofuran moiety of Compound B at one end of the pocket, adjacent to the catalytic zinc or the opposite end, distant from the zinc atom. Property analysis of the enzymes S1' pocket depicts that the end adjacent to the zinc is relatively
- 20 polar whereas the opposite end is hydrophobic. This analysis lead us to dock Compound B with the morpholine ring adjacent to the catalytic zinc atom with the benzofuran moiety siting in a hydrophobic pocket formed by L115, L136, F149 and P152 at the base of the S1' pocket. To further verify the proposed binding of Compound B in the S1' pocket of MMP-13, a simple competition
- 25 experiment with Compound A was conducted. The ^1H - ^{15}N HSQC experiment for the MMP-13:Compound B complex was collected in the presence of Compound A. The presence of Compound A displaced all of Compound B as evident by the distinct differences in the ^1H - ^{15}N HSQC spectra which further suggests that both compounds bind in the S1' pocket.
- 30 The relative orientation and binding of Compound B with MMP-13 was further confirmed by the observation of intermolecular NOEs between

-58-

Compound B and MMP-13 from the 3D ^{13}C -edited/ ^{12}C -filtered NOESY experiment. The NOESY spectra was collected in the presence of a ten-fold excess of Compound B because of the weak affinity of Compound B with MMP-13. Nevertheless, a total of 16 NOEs were observed between Compound B and

5 L81, L115, V116, Y141, T142 and Y143 which support the initial positioning of Compound B in the MMP-13 S1' pocket. An expanded 2D plane from the 3D ^{13}C -edited/ ^{12}C -filtered NOESY experiment (not shown) demonstrated examples of some key intermolecular NOEs between Compound B benzofuran group resonances and L115 δ and Compound B resonances proximal to the

10 morpholine ring and L82 δ . The complex of Compound B with MMP-13 was subjected to energy refinement using the NMR results as constraints (Moy, *et al.*, Biochemistry 1999; Chen, *et al.*, J. Biomol. Struct. Dyn. 1995). The modeling results depict the morpholine oxygen forming a hydrogen bond with the backbone amide group of Leu-82 and the benzofuran group packs deep in

15 the S1' pocket with the peptide bond linker portion forming hydrogen bonds with protein backbone groups. The complex shows no apparent interactions between the inhibitor and the catalytic zinc justifying the ligands micromolar potency.

20 *Structures of MMP-1, MMP-9 and MMP-13:* The recent NMR solution structures of MMP-1 and MMP-13 were used as starting points for molecular modeling and analysis (Moy, *et al.*, Biochemistry Submitted 1999; Moy, *et al.*, Biochemistry 1998; Moy, *et al.*, Biochemistry 1999). A homology model for MMP-9 was developed based on its strong homology to MMP-1 (54% identity around the

25 catalytic domain). Based on the homology model, the catalytic site of MMP-9 is similar to the corresponding sites in MMP-1 and MMP-13. All three structures were used as starting points for analysis and synthetic design.

Comparative analysis of the MMP structures shows that residue positions 115 and 144, in addition to the length of the specificity loop,

30 determines the size and shape of the S1' pockets. Alignment of the NMR structures for MMP-1 and MMP-13 shows that MMP-13 contains two additional

insertions in the specificity loop. The homology model of MMP-9 indicates no additional insertions so its length is identical to MMP-1.

Residue positions 115 and 144 are important in establishing the relative length of the S1' pockets for the MMPs where the larger the side chain at these positions results in a smaller S1' pocket. Since residue 115 is spatially closer to the catalytic zinc than residue 144, a larger side chain for residue 115 will have a greater impact on defining a smaller S1' pocket compared to residue 144. MMP-1 has the largest side chain at position 115, thus its S1' pocket is the smallest. MMP-9 has an Arg at position 144 resulting in its S1' pocket being longer compared to MMP-1. Conversely, MMP-13 has short side chains at both positions 115 and 144. The short side chains combined with an increased length of its specificity loop result in MMP-13 having the largest S1' pocket. To summarize, the size of the MMP S1' pockets are as follows: MMP-13 > MMP-9 > MMP-1 where this structural feature plays a critical role in the design strategy for developing a potent and specific MMP-13 inhibitor.

Design Strategy: A strategy utilizing NMR and molecular modeling was applied towards the design and synthesis of an MMP-13 selective inhibitor lead. The basic approach behind the design strategy is to optimize the affinity of the chemical lead Compound B while maintaining its inherent MMP-13 selectivity. This can be achieved by taking advantage of the distinct structural feature of MMP-13, its deep linear S1' pocket, while combining overlapping structural features of Compound B with other potent inhibitors. Compound C is an example of a potent and selective inhibitor for MMP-9 and MMP-13 (See Table 2). Based on the NMR solution structure of MMP-13 complexed with Compound A (Figure 4), structurally similar inhibitors were positioned into the active site of MMP-13.

Figure 7 shows the critical regions of Compound C, which can be broken down into two components, Compound D which represents the zinc chelating portion of the compound that contributes to the binding potency and the toluene group (1A) which contributes to enhanced ligand selectivity against

MMP-1. The strategy was to design a new inhibitor based on replacing the toluene group (1A) with a component of Compound B critical for binding within the extended S1' pocket of MMP-13. The overlay of the NMR solution structure for Compound B with the model for Compound D is shown in Figure 8B. The close similarity between the positioning of the two structures made it readily apparent that it would be possible to generate a hybrid of the two structures combining the potent Compound D with the selective component of Compound B (Figure 8A). These results were then used to design the proposed hybrid inhibitor Compound E. The assay data in Table 2 clearly shows that the new inhibitor, Compound E, has better potency compared to Compound C in addition to improved selectivity towards MMP-13. Thus, the combination of NMR spectroscopy with molecular modeling techniques resulted in the design of a novel, potent and selective MMP-13 inhibitor (Compound E) which has an IC₅₀ of 17 nM for MMP-13 and showed >5800, 56 and >500 fold selectivity against MMP-1, MMP-9 and TACE, respectively. To the best of our knowledge, this represents the first example of a potent MMP-13 inhibitor that has been shown to be selective against MMP-9.

Table 2 - IC50 and Selectivity Data

| 20 | Compound | MMP-1 | MMP-9 | MMP-13 | TACE | S-1 ^a | S-9 ^a | S-TACE ^a |
|----|--|--------|-------|--------|-------|------------------|------------------|---------------------|
| | C | 750nM | 46nM | 75nM | 470nM | 10.0x | 0.6x | 6.3x |
| | D | 82nM | 21nM | 15nM | 240nM | 5.5x | 1.4x | 16x |
| | E | NA | 945nM | 17nM | 19% | >5800x | 56x | >500x |
| | F | 1025nM | 71nM | 301nM | 664nM | 3.4x | 0.2x | 2.2x |
| 25 | ^a Selectivity data presented as a ratio of the MMP or TACE IC ₅₀ with MMP-13 | | | | | | | |

-61-

Example 4

The X-ray crystal structure of the MMP-13:Compound A complex was determined using the following procedure:

- 5 *Gene/expression system/production:* The cDNA coding for human MMP-13 proenzyme had 85 residues of the PRO domain, followed by 165 residues of the catalytic domain (CAT). The gene was carried on a pET-21a expression plasmid, under the control of a bacteriophage T7 promoter. The expression host was *Escherichia coli* BL21(DE3), which had a chromosomal copy of T7 RNA
10 polymerase under *lac* control. Cells were grown in nutrient broth, and synthesis of PRO-CAT was induced by isopropyl- β -thiogalactoside. The protein accumulated to 5-10% of total cellular protein, essentially all of which was aggregated into inclusion bodies.

- For potential MAD experiments, the plasmid was transferred into a
15 methionine auxotroph host. PRO-CAT with selenomethionine substitution was produced by induction in a defined medium, with methionine replaced by selenomethionine.

- Purification and refolding of PRO-CAT:* Frozen cells were disrupted
20 mechanically, and inclusion bodies were isolated by centrifugation. PRO-CAT was solubilized with urea containing dithiothreitol to disrupt any disulfide bridges. PRO-CAT was partially purified by anion-exchange chromatography, in urea, on Q Sepharose. The protein was diluted to about 400 μ g/ml in a solution of sodium chloride, calcium chloride, and zinc acetate, buffered with
25 tricine-HCl. Refolding proceeded over 3-4 days, during dialysis, with multiple buffer changes. PRO-CAT was then concentrated for activation and release of CAT.

- Activation of PRO-CAT:* The presently-accepted view of MMPs holds that the
30 proenzyme form is maintained in an inactive state through the coordination of one cysteine from the PRO domain into the active-site zinc. If this cysteine is

-62-

displaced, the enzyme becomes active. In our protocol, aminophenyl mercuric acetate was added to the protein solution to form a mercurial adduct with the cysteine. Progress of activation was monitored by SDS polyacrylamide gel electrophoresis. Results indicated that the CAT domain accumulated and the
5 PRO domain was degraded to small peptides.

Purification of MMP-13 (CAT) – Size Exclusion: Following activation and PRO cleavage, MMP-13 was isolated by size-exclusion chromatography through SuperDex 75 in a solution of sodium chloride, calcium chloride, and zinc
10 acetate, buffered with tris-HCl.

Purification of MMP-13 – Affinity: MMP-13 was further purified by affinity chromatography on an immobilized hydroxamate inhibitor. The affinity matrix was prepared by coupling an hydroxamate inhibitor to Sepharose through the
15 amino group of the piperazine ring. MMP-13 can be absorbed to the matrix and desorbed by displacement using another inhibitor of choice.

Characterization of MMP-13: Protein preparations for crystallization trials were validated by several techniques. Routinely, SDS-PAGE showed a predominant
20 species whose migration was consistent with a molecular weight of around 19,000. MALDITOF mass spectroscopy demonstrates a single species consistent with the expected size of 18,588 amu. (MMP-13 prepared with selenomethionine showed essentially complete replacement). N-terminal sequencing demonstrated that the protein begins with YNVF, as expected for
25 correct cleavage between PRO and CAT. Retention volume in analytical size-exclusion chromatography was consistent with a monomeric protein: no detectable aggregation was observed. The final protein was enzymatically active on a fluorogenic peptide substrate, and degraded denatured collagen.

30 *Crystallization of MMP-13 complex with Compound A:* The MMP-13 protein solution was buffered with 10 mM tris-HCL buffer, pH 7.5, and 0.25 M NaCl.

-63-

The concentration of protein used for crystallization was 20.0 mg/ml. The inhibitor solution was added to a protein solution with a mole ratio (protein:inhibitor) of 1:2, and was mixed for more than 1 hour.

Crystallization conditions were screened by the hanging-drop vapor diffusion method (McPherson, A., Methods Biochem. Anal. 1976). A successful procedure for growing crystals of this complex at room temperature was identified, and crystals were obtained. Specifically, a solution was prepared from 3 μ l of protein solution and 3 μ l of precipitant solution, which consisted of 26% PEG4000, 0.1 M ammonium sulfate, and 0.1 M sodium chloride. A drop of this solution was suspended on a microscope coverslip glass which had been coated with silicone to prevent drop spreading. The reservoir solutions consisted of 0.6 ml precipitant solution. Equilibration was performed at room temperature by vapor diffusion. Crystals began appearing after three days. After two weeks, these crystals stopped growing. The X-ray data which have been processed show that the MMP-13 complex was crystallized in two forms. One crystal form is C-centered orthorhombic; it belonged to space group C2221, and had a cell dimension of $a=36.3 \text{ \AA}$, $b=134.4 \text{ \AA}$, and $c=134.8 \text{ \AA}$. This crystal had high mosaicity; therefore, it would be of little use when working on the structure of the complex. The second crystal form is primitive orthorhombic, from space group P21212, with a cell constant of $a=108.3 \text{ \AA}$, $b=79.8 \text{ \AA}$, and $c=36.1 \text{ \AA}$. This crystal had low mosaicity, but it was very small in most cases.

In order to obtain a big single crystal for X-ray data collections, the seeding technique (Thaller, C., et al., J. Mol. Biol. 1981) was applied. This was accomplished by using both the microseeding and the macroseeding methods. Small seed crystals were transferred to a 20% PEG4000 precipitant solution on a depression slide. A single washed crystal was injected into a hanging-drop solution, which was composed of 3 μ l of MMP-13 complex solution and 3 μ l of precipitant solution. The reservoir solutions consisted of 0.6 ml precipitant solution at pH 8.0. This procedure successfully produced bigger crystals with a maximum edge dimension of up to $0.35 \times 0.1 \times 0.1 \text{ mm}^3$. These crystals diffracted X-ray at a resolution of 2.0 \AA .

-64-

X-Ray Data Collection: X-ray diffraction data from 30.0-2.0 Å resolution for the MMP-13:Compound A complex crystal (P21212 form) was collected by using an RAXIS IIC Image Plate area detector which used graphite monochromatic CuKα radiation from a Rigaku RU200 rotating anode generator (operating at 50 kV, 100 mA) at a low temperature of 100 K. The oscillation angle for each plate was 1 degree, and exposure time was 20 minutes per 'image'. The processing of X-ray diffraction data was accomplished using the HKL programs (Otwinowski, Z. and Minor, W., Methods in Enzymology 276:307-26). The R-merges for full and partial reflections were 4.0% and 6.04% respectively. 18,782 unique reflections (81% complete at 2.0 Å resolutions) were collected.

Structure Determination and Refinement: The MMP-13 complex crystal structure has been determined by a combination of crystallographic modeling and the Molecular Replacement method using models of MMP-13 derived from the MMP-1 and MMP-8 structures. The homology between MMP-13 and MMP-8 is 56% by sequence, and at least 70% by structure. Crystals of the MMP-13 complex have two molecules in the asymmetric unit, i.e., the unit is a dimer. Conventional molecular replacement was not effective for determination of this dimer structure by using a monomer model. There are two reasons for this: (1) the high symmetry of the crystal structure; and (2) the conformations and the configurations of the side chain and the main chain in flexible loops of MMP-13 and MMP-8.

Firstly, the crystal structure of the MMP-13 complex is highly symmetrical. The P21212 crystal has four symmetry operations, and there are eight molecules in a unit cell. A second crystal form, belonging to space group C222, and having eight symmetry operations in a unit cell, has been identified. In this crystal, there are 16 monomers per cell in the dimer structure, and 32 monomers per cell in the tetramer structure. Therefore, the rotation search and especial translation search become more difficult. Secondly, even though the MMP family's catalytic domain structure is highly conserved, the conformations and the configurations of the side chain and the main chain in flexible loops of

-65-

MMP-13 and MMP-8 may not be the same. In particular, the similarity between the two structures may not be sufficient to permit the determination of the dimer structure using a monomer as the searching model.

Many attempts at a rotation and translation search were made by
5 using the X-ray data and models of either a monomer of MMP-8 or a dimer of MMP-1. Some rotation solutions were obtained, but no final translation solution has been found by using the monomer model. Accordingly, to determine this structure, it was proposed that a dimer model be constructed first; the molecular replacement method was then applied to solve the structure.

10 The key idea of this proposal was crystal packing. To construct a dimer, the orientations of each monomer were determined on the basis of a rotation search. The positions of each monomer were located on the basis of the molecular packing in unit cell. Many dimer models have been constructed and applied as the 'model' for searching the rotation and translation using
15 program AMORE (Collaborative Computational Project, Number 4 (CCP4) (1994), Acta Cryst. D50:760-763). One dimer model was found to be correct, and finally resulted in the MMP-13 3-D crystal structure using the molecular replacement method. The MMP-13 complex structure was confirmed by observing the most important and significant fact that the positions of the two
20 zinc ions and the two calcium ions could be identified from the difference ($F_o - F_c$) maps with five-sigma cut, where F_o was observed structure factor and F_c was the calculated structure factor of the dimer model without zinc and calcium atoms.

These ions were located in the exact positions where they were
25 observed in other MMP family members. The molecule fits the ($2F_o - F_c$) electron densities very well, both in main chain and in side chain. The molecule fits the $2F_o - F_c$ electron density quite well. All of these MMP molecules are conserved in the core structure region, especially the position of the central helix and the catalytic zinc. The MMP-13 dimer structure was further confirmed
30 by applying the molecular replacement programs XPLOR (Brünger, A.T., XPLOR Version 3.1 Manual, Yale University, New Haven CT) and MERLOT (Fitzgerald,

-66-

P., MERLOT, version 2.4 (Nov. 10, 1991). All of them worked very well, and produced results which were in agreement with the MMP-13 structure.

Structure Refinement: The structure refinement was carried out by the program
5 XPLOR. The initial dimer model included 320 amino acid residues without zinc
and calcium ions. The dimer model was refined against 2.0 Å X-ray data,
collected on an RAXIS IIC area detector at a temperature of 100 K. The progress
of the refinement was evaluated from the quality of the protein molecular
conformations and the electron density maps, and the values of the
10 crystallographic R-factor. The initial R-factor was 52%. After rigid-body
minimization, conjugated-gradient minimization, a heating stage, a slow-cooling
stage in the range from 4000K to 300K, energy minimization, B-factor
refinement, and positional refinement, the R-factor lowered to 0.32. Electron-
density maps with coefficients of (2Fo-Fc) and (Fo-Fc), as well as the phases,
15 were calculated. The difference map shows four zinc ions and four calcium ions
in the dimer structure with five-sigma cut. Some side chain loops and a few
main loops were rebuilt on the interactive graphics system. The rebuilt dimer
plus the zinc and calcium ions, as the new model, was refined. The R-factor
was down to 26.6%. At this stage, a model of inhibitor Compound A was
20 positioned in the active-site region based on the difference electron density.

The complex structure was refined by repeating the above steps,
with the R-factor down to 20%. The water molecules were modeled as oxygen
atoms. Their initial positions were located by searching the peaks in the (Fo-Fc)
difference maps. These positions were then checked by calculating the distance
25 between 'water' and the oxygen and nitrogen of the protein. Together with the
protein (complex) atoms, these 'water' molecules were refined against the X-ray
data. Once the temperature factor of water was higher than 50, this water was
omitted. 120 water molecules near the protein were found, and five water
molecules were identified in the active site of each monomer. The (2Fo-Fc)
30 maps were used to adjust the solvent model and to aid in the placement of new
solvent molecules, as well as to check and correct the whole model. The r.m.s.

-67-

deviations of C α atoms for bond angles and bond distances from ideal geometry were 1.6° and 0.012 Å. The final crystallographic R-factor was 22%, at a resolution of 2.0 Å.

All publications mentioned herein above, whether to issued

5 patents, pending applications, published articles, protein structure deposits, or otherwise, are hereby incorporated by reference in their entirety. While the foregoing invention has been described in some detail for purposes of clarity and understanding, it will be appreciated by one skilled in the art from a reading of the disclosure that various changes in form and detail can be made

10 without departing from the true scope of the invention in the appended claims.

What is claimed is:

1. A solution comprising a biologically active catalytic fragment of human collagenase-3 (MMP-13) complexed with N-Hydroxy-2-[(4-methoxy-benzenesulfonyl)-pyridin-3-ylmethyl-amino]-3-methyl-benzamide ("Compound A").
2. The solution of Claim 1, wherein the catalytic fragment of MMP-13 comprises the amino acid residues of Figure 1.
3. The solution of Claim 2, comprising 1 mM MMP-13 complexed with Compound A in a 1:1 molar ratio, in a buffer comprising 10mM deuterated Tris-Base, 100mM NaCl, 5mM CaCl₂, 0.1mM ZnCl₂, 2mM NaN₃, and 10 mM deuterated DTT in either 90% H₂O/10% D₂O or 100% D₂O.
4. The solution of Claim 3, wherein the MMP-13 is either ¹⁵N enriched or ¹⁵N, ¹³C enriched.
5. The solution of Claim 1, wherein the secondary structure of the catalytic fragment of MMP-13 comprises three alpha helices and a mixed parallel and anti-parallel beta sheet comprising five beta strands.
6. The solution of Claim 5, wherein the alpha helices and beta strands are configured in the order β_I , α_A , β_{II} , β_{III} , β_{IV} , β_V , α_B , and α_C .
7. The solution of Claim 6, wherein the three alpha helices correspond to residues 28-44 (α_A), 112-123 (α_B) and 153-163 (α_C) of Figure 1, and the five beta strands correspond to residues 83-86 (β_I), 95-100 (β_{II}), 59-66 (β_{III}), 14-20 (β_{IV}), and 49-53 (β_V) of Figure 1.
8. A crystallized catalytic fragment of MMP-13 complexed with N-Hydroxy-2-[(4-methoxy-benzenesulfonyl)-pyridin-3-ylmethyl-amino]-3-

-69-

methyl-benzamide ("Compound A").

9. The crystallized complex of Claim 8, wherein the catalytic fragment of MMP-13 comprises the amino acid residues of Figure 1.

10. The crystallized complex of Claim 9, characterized as being in orthorhombic form with space group P21212, and having unit cell parameters of $a=108.3\text{\AA}$, $b=79.8\text{\AA}$, and $c=36.1\text{\AA}$.

11. The crystallized complex of Claim 10, further characterized as consisting of two molecules of MMP-13:Compound A complex in the asymmetric unit.

12. The crystallized complex of Claim 11, wherein the secondary structure of the catalytic fragment of MMP-13 comprises three alpha helices and a mixed parallel and anti-parallel beta sheet comprising five beta strands.

13. The crystallized complex of Claim 12, wherein the alpha helices and beta strands are configured in the order β_I , α_A , β_{II} , β_{III} , β_{IV} , β_V , α_B , and α_C .

14. The crystallized complex of Claim 13, wherein the three alpha helices correspond to residues 28-44 (α_A), 112-123 (α_B) and 153-163 (α_C) of Figure 1, and the five beta strands correspond to residues 83-86 (β_I), 95-100 (β_{II}), 59-66 (β_{III}), 14-20 (β_{IV}), and 49-53 (β_V) of Figure 1.

15. An active site of MMP-13, characterized by a catalytic zinc, a beta strand, a Ca^{2+} binding loop, an alpha helix, and a random coil region.

-70-

16. The active site of Claim 15, wherein the beta strand comprises residues N14, L15, T16, Y17, R18, I19, and V20 according to Figure 1, the Ca^{2+} binding loop comprises residues F75, D76, G77, P78, and S79 according to Figure 1, the alpha helix comprises residues N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, and H123 according to Figure 1, and the random coil region comprises residues P139, I140, and Y141 according to Figure 1.

17. The active site of Claim 16, wherein said active site comprises the relative structural coordinates of the catalytic zinc and amino acid residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, \pm a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å.

18. The active site of Claim 17, further comprising the relative structural coordinates of amino acid residues G80, L81, L82, A83, H84, A85, K109, G110, Y111, S124, L125, G126, L127, D128, H129, S130, K131, D132, P133, G134, A135, L136, M137, F138, T142, Y143, T144, and G145 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, \pm a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5Å.

19. The active site of Claim 18, further comprising the relative structural coordinates of amino acid residues F149 and P152 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, \pm a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5Å.

-71-

20. An active site of MMP-13 comprising the relative structural coordinates of a catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, \pm a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å.

21. A method for identifying a potential inhibitor or activator of MMP-13, comprising the steps of:

(a) using a three dimensional structure of MMP-13 as defined by the relative structural coordinates of amino acids encoding MMP-13 according to Figures 4 or 5, \pm a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5Å;

(b) employing said three-dimensional structure to design or select a potential inhibitor or activator; and

(c) synthesizing or obtaining said potential inhibitor or activator.

22. The method according to Claim 21, wherein the potential inhibitor is designed de novo.

23. The method according to Claim 21, wherein the potential inhibitor is designed from a known inhibitor.

24. The method of Claim 22, further comprising the step of contacting the potential inhibitor with MMP-13 in the presence of a substrate to determine the ability of the potential inhibitor to inhibit MMP-13.

25. The method of Claim 23, further comprising the step of contacting the potential inhibitor with MMP-13 in the presence of a substrate to determine the ability of the potential inhibitor to inhibit MMP-13.

-72-

26. The method according to Claim 21, wherein the step of employing the three dimensional structure to design or select the potential inhibitor comprises the steps of:

- (a) identifying chemical entities or fragments capable of associating with MMP-13; and
- (b) assembling the identified chemical entities or fragments into a single molecule to provide the structure of the potential inhibitor.

27. The method according to Claim 26, wherein the potential inhibitor is designed de novo.

28. The method according to Claim 26, wherein the potential inhibitor is designed from a known inhibitor.

29. The method of Claim 27, further comprising the step of contacting the potential inhibitor with MMP-13 in the presence of a substrate to determine the ability of the potential inhibitor to inhibit MMP-13.

30. The method of Claim 28, further comprising the step of contacting the potential inhibitor with MMP-13 in the presence of a substrate to determine the ability of the potential inhibitor to inhibit MMP-13.

31. An inhibitor identified or designed by the method of Claim 21.

32. An inhibitor identified or designed by the method of Claim 26.

1 / 75

| | | | | |
|--------------|--------------|--------------|--------------|--------------|
| YNVFP 5 | RTLKW 10 | SKMNL 15 | TYRJV 20 | NYTPD 25 |
| MTHSE 30 | VEKAF 35 | KKAFK 40 | VWSDV 45 | TPLNF 50 |
| TRLHD 55 | GIADI 60 | MISFG 65 | IKEHG 70 | DFYPF 75 |
| DGPSG 80 | LLAHA 85 | FPPGP 90 | NYGGD 95 | AHFDD 100 |
| DETWT 105 | SSSKG 110 | YNLFL 115 | VAAHE 120 | FGHSL 125 |
| GLDHS 130 | KDPGA 135 | LMFPI 140 | YTYTG 145 | KSHFM 150 |
| LPDDD 155 | VQGIQ 160 | SLYG 164 | | |

FIG. 1

2 / 75

Sequence 1: MMP-13

Sequence 2: MMP-1

Identity score: 58.9 %

VGEYNVFPRTLKWSKMNLTYRIVNYTPDMTHSEVEKAFKKAFFVWSDVTPLNFTRLHDGIADIMISFGIKEHGDFFYFDG
LTEGN PR WEQTHLTYRIENYTPDLPRADVDAIEKAFQLWSNVTPLTFTKVSEGQADIMISFVRGDHRDNSPFDG

PSGLLAHAFFPGPNYGGDAHFDDDETWS SSKGYNLF LVAAHEFGHSLGLDHSKDPGALMF
PIYTYTGKSHFMLPDDDVQ
PGGNLAHAFFQPGGIGGDAHFDEDERWTNNFREYNLHRVAAHELGHSGLS HST DIGALMYPSYTFSGDVQ LAODD
ID

###

GIQSLYGPGEDEPN
GIQAIYQRSQ

FIG. 2A

Sequence 1: MMP-13

Sequence 2: MMP-8

Identity score: 61.4 %

VGEYNVFPRTLKWSKMNLTYRIVNYT PDMTH S EVEKAFKKAFFVWSDVTPLNFTRLHDGIADIMISFGIKEHGDFFYFDG
NPKWER T NLTYRIRNYTP QLSEA EVERAI KDAFEL WSVASPLI
FTRISQGEADINIAFYQRDHGDNSPFDG

..

PSGLLAHAFFPGPNYGGDAHFDDDETWTSSSKGYNLFLVAAHEFGHSLGLDHSKDPGALMF PIYTYTGKSHFMLPDDDVQ
PNGILAHAFQPGQGIGGDAHFDAEETWTNTSANYNLFLVAA HEFGHSLGLAHSSDPGALMYPNYAE RETSNYSLPDD ID
###

GIQSLYGPGEDEPN
GIQAIYG

FIG. 2B

3/ 75

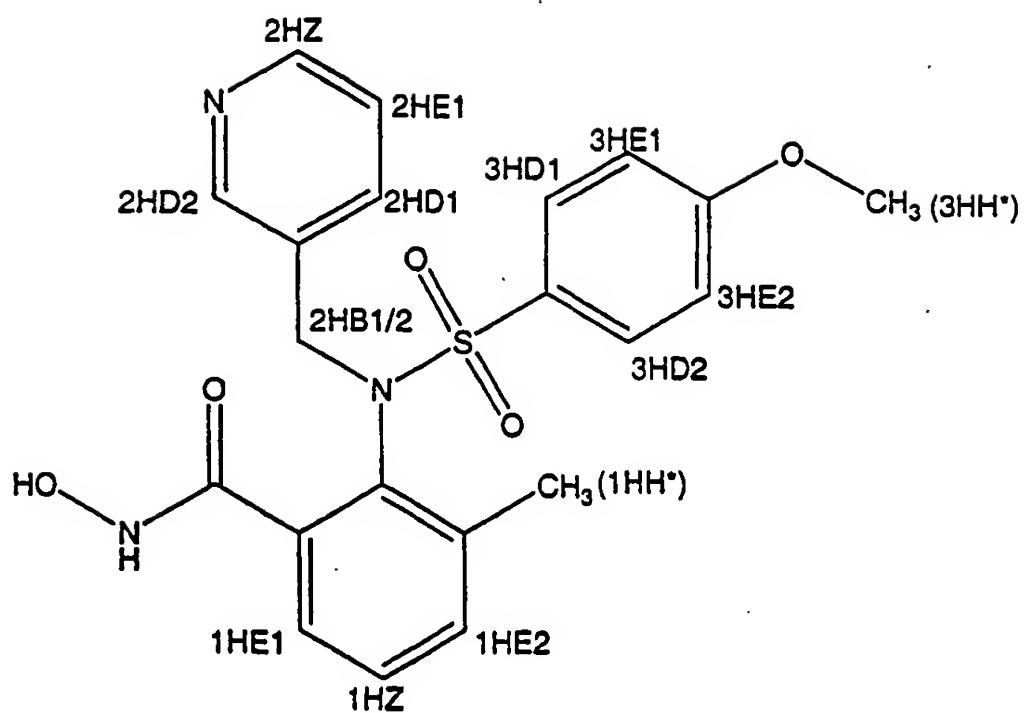


FIG. 3

4/75

| | Atom Type | Res. | | X | Y | Z | | |
|------|--------------|------|---|---------|---------|---------|------|------|
| ATOM | 1 N | THR | 7 | -12.675 | -13.911 | -8.815 | 1.00 | 0.83 |
| ATOM | 2 HN | THR | 7 | -12.001 | -14.254 | -8.192 | 1.00 | 1.22 |
| ATOM | 3 CA | THR | 7 | -14.063 | -13.649 | -8.340 | 1.00 | 0.63 |
| ATOM | 4 HA | THR | 7 | -14.744 | -14.330 | -8.830 | 1.00 | 0.73 |
| ATOM | 5 CB | THR | 7 | -14.132 | -13.858 | -6.825 | 1.00 | 0.61 |
| ATOM | 6 HB | THR | 7 | -13.473 | -13.158 | -6.335 | 1.00 | 0.66 |
| ATOM | 7 OG1 | THR | 7 | -13.730 | -15.185 | -6.514 | 1.00 | 0.71 |
| ATOM | 8 HG1 | THR | 7 | -13.721 | -15.690 | -7.330 | 1.00 | 1.07 |
| ATOM | 9 CG2 | THR | 7 | -15.564 | -13.628 | -6.336 | 1.00 | 0.67 |
| ATOM | 10 HG21 | THR | 7 | -15.712 | -12.577 | -6.139 | 1.00 | 1.14 |
| ATOM | 11 HG22 | THR | 7 | -15.728 | -14.191 | -5.429 | 1.00 | 1.32 |
| ATOM | 12 HG23 | THR | 7 | -16.261 | -13.955 | -7.093 | 1.00 | 1.23 |
| ATOM | 13 C | THR | 7 | -14.451 | -12.208 | -8.678 | 1.00 | 0.52 |
| ATOM | 14 O | THR | 7 | -15.416 | -11.962 | -9.374 | 1.00 | 0.65 |
| ATOM | 15 N | LEU | 8 | -13.704 | -11.254 | -8.195 | 1.00 | 0.47 |
| ATOM | 16 HN | LEU | 8 | -12.927 | -11.473 | -7.639 | 1.00 | 0.61 |
| ATOM | 17 CA | LEU | 8 | -14.027 | -9.831 | -8.495 | 1.00 | 0.42 |
| ATOM | 18 HA | LEU | 8 | -15.098 | -9.715 | -8.575 | 1.00 | 0.43 |
| ATOM | 19 CB | LEU | 8 | -13.495 | -8.937 | -7.370 | 1.00 | 0.52 |
| ATOM | 20 HB1 | LEU | 8 | -13.721 | -7.905 | -7.591 | 1.00 | 0.54 |
| ATOM | 21 HB2 | LEU | 8 | -12.424 | -9.060 | -7.292 | 1.00 | 0.58 |
| ATOM | 22 CG | LEU | 8 | -14.151 | -9.331 | -6.042 | 1.00 | 0.60 |
| ATOM | 23 HG | LEU | 8 | -13.958 | -10.376 | -5.844 | 1.00 | 0.60 |
| ATOM | 24 CD1 | LEU | 8 | -13.566 | -8.484 | -4.910 | 1.00 | 0.74 |
| ATOM | 25 HD11 | LEU | 8 | -13.899 | -8.875 | -3.960 | 1.00 | 1.22 |
| ATOM | 26 HD12 | LEU | 8 | -13.900 | -7.462 | -5.016 | 1.00 | 1.26 |
| ATOM | 27 HD13 | LEU | 8 | -12.488 | -8.518 | -4.956 | 1.00 | 1.31 |
| ATOM | 28 CD2 | LEU | 8 | -15.664 | -9.096 | -6.117 | 1.00 | 0.61 |
| ATOM | 29 HD21 | LEU | 8 | -15.871 | -8.278 | -6.791 | 1.00 | 1.13 |
| ATOM | 30 HD22 | LEU | 8 | -16.040 | -8.856 | -5.134 | 1.00 | 1.18 |
| ATOM | 31 HD23 | LEU | 8 | -16.149 | -9.991 | -6.478 | 1.00 | 1.26 |
| ATOM | 32 C | LEU | 8 | -13.374 | -9.438 | -9.822 | 1.00 | 0.40 |
| ATOM | 33 O | LEU | 8 | -12.218 | -9.722 | -10.064 | 1.00 | 0.45 |
| ATOM | 34 N | LYS | 9 | -14.109 | -8.795 | -10.687 | 1.00 | 0.36 |
| ATOM | 35 HN | LYS | 9 | -15.042 | -8.581 | -10.474 | 1.00 | 0.36 |
| ATOM | 36 CA | LYS | 9 | -13.536 | -8.393 | -12.002 | 1.00 | 0.37 |
| ATOM | 37 HA | LYS | 9 | -12.521 | -8.050 | -11.862 | 1.00 | 0.39 |
| ATOM | 38 CB | LYS | 9 | -13.539 | -9.599 | -12.944 | 1.00 | 0.50 |
| ATOM | 39 HB1 | LYS | 9 | -12.851 | -10.344 | -12.573 | 1.00 | 0.60 |

FIG. 4

5/75

| | | | | | | | | | |
|------|-----|-----|-----|----|---------|---------|---------|------|------|
| ATOM | 40 | HB2 | LYS | 9 | -13.233 | -9.286 | -13.932 | 1.00 | 0.48 |
| ATOM | 41 | CG | LYS | 9 | -14.948 | -10.193 | -13.007 | 1.00 | 0.60 |
| ATOM | 42 | HG1 | LYS | 9 | -15.632 | -9.455 | -13.398 | 1.00 | 0.66 |
| ATOM | 43 | HG2 | LYS | 9 | -15.260 | -10.482 | -12.014 | 1.00 | 0.78 |
| ATOM | 44 | CD | LYS | 9 | -14.951 | -11.421 | -13.921 | 1.00 | 0.94 |
| ATOM | 45 | HD1 | LYS | 9 | -13.944 | -11.794 | -14.033 | 1.00 | 1.57 |
| ATOM | 46 | HD2 | LYS | 9 | -15.344 | -11.147 | -14.889 | 1.00 | 1.62 |
| ATOM | 47 | CE | LYS | 9 | -15.829 | -12.511 | -13.303 | 1.00 | 0.57 |
| ATOM | 48 | HE1 | LYS | 9 | -16.776 | -12.086 | -13.007 | 1.00 | 1.15 |
| ATOM | 49 | HE2 | LYS | 9 | -15.333 | -12.924 | -12.437 | 1.00 | 1.10 |
| ATOM | 50 | NZ | LYS | 9 | -16.060 | -13.591 | -14.304 | 1.00 | 1.61 |
| ATOM | 51 | HZ1 | LYS | 9 | -15.181 | -14.127 | -14.445 | 1.00 | 2.14 |
| ATOM | 52 | HZ2 | LYS | 9 | -16.358 | -13.168 | -15.207 | 1.00 | 2.13 |
| ATOM | 53 | HZ3 | LYS | 9 | -16.802 | -14.231 | -13.959 | 1.00 | 2.14 |
| ATOM | 54 | C | LYS | 9 | -14.377 | -7.265 | -12.605 | 1.00 | 0.32 |
| ATOM | 55 | O | LYS | 9 | -15.493 | -7.021 | -12.191 | 1.00 | 0.34 |
| ATOM | 56 | N | TRP | 10 | -13.850 | -6.571 | -13.577 | 1.00 | 0.31 |
| ATOM | 57 | HN | TRP | 10 | -12.947 | -6.781 | -13.895 | 1.00 | 0.33 |
| ATOM | 58 | CA | TRP | 10 | -14.618 | -5.456 | -14.201 | 1.00 | 0.30 |
| ATOM | 59 | HA | TRP | 10 | -15.030 | -4.826 | -13.427 | 1.00 | 0.29 |
| ATOM | 60 | CB | TRP | 10 | -13.684 | -4.630 | -15.088 | 1.00 | 0.29 |
| ATOM | 61 | HB1 | TRP | 10 | -14.264 | -3.917 | -15.655 | 1.00 | 0.32 |
| ATOM | 62 | HB2 | TRP | 10 | -13.157 | -5.286 | -15.765 | 1.00 | 0.33 |
| ATOM | 63 | CG | TRP | 10 | -12.699 | -3.901 | -14.230 | 1.00 | 0.25 |
| ATOM | 64 | CD1 | TRP | 10 | -11.516 | -4.405 | -13.812 | 1.00 | 0.30 |
| ATOM | 65 | HD1 | TRP | 10 | -11.137 | -5.390 | -14.040 | 1.00 | 0.37 |
| ATOM | 66 | CD2 | TRP | 10 | -12.786 | -2.553 | -13.683 | 1.00 | 0.21 |
| ATOM | 67 | NE1 | TRP | 10 | -10.872 | -3.454 | -13.042 | 1.00 | 0.30 |
| ATOM | 68 | HE1 | TRP | 10 | -9.996 | -3.569 | -12.617 | 1.00 | 0.36 |
| ATOM | 69 | CE2 | TRP | 10 | -11.614 | -2.295 | -12.934 | 1.00 | 0.23 |
| ATOM | 70 | CE3 | TRP | 10 | -13.758 | -1.538 | -13.763 | 1.00 | 0.24 |
| ATOM | 71 | HE3 | TRP | 10 | -14.663 | -1.706 | -14.328 | 1.00 | 0.29 |
| ATOM | 72 | CZ2 | TRP | 10 | -11.412 | -1.075 | -12.287 | 1.00 | 0.22 |
| ATOM | 73 | HZ2 | TRP | 10 | -10.509 | -0.903 | -11.720 | 1.00 | 0.27 |
| ATOM | 74 | CZ3 | TRP | 10 | -13.558 | -0.309 | -13.113 | 1.00 | 0.25 |
| ATOM | 75 | HZ3 | TRP | 10 | -14.310 | 0.463 | -13.181 | 1.00 | 0.32 |
| ATOM | 76 | CH2 | TRP | 10 | -12.387 | -0.078 | -12.376 | 1.00 | 0.23 |
| ATOM | 77 | HH2 | TRP | 10 | -12.238 | 0.870 | -11.879 | 1.00 | 0.26 |
| ATOM | 78 | C | TRP | 10 | -15.755 | -6.031 | -15.050 | 1.00 | 0.39 |
| ATOM | 79 | O | TRP | 10 | -15.641 | -7.098 | -15.620 | 1.00 | 0.48 |
| ATOM | 80 | N | SER | 11 | -16.855 | -5.332 | -15.132 | 1.00 | 0.43 |
| ATOM | 81 | HN | SER | 11 | -16.927 | -4.476 | -14.660 | 1.00 | 0.44 |
| ATOM | 82 | CA | SER | 11 | -18.006 | -5.835 | -15.936 | 1.00 | 0.52 |
| ATOM | 83 | HA | SER | 11 | -18.003 | -6.915 | -15.930 | 1.00 | 0.59 |
| ATOM | 84 | CB | SER | 11 | -19.313 | -5.330 | -15.325 | 1.00 | 0.64 |
| ATOM | 85 | HB1 | SER | 11 | -19.120 | -4.425 | -14.763 | 1.00 | 1.16 |
| ATOM | 86 | HB2 | SER | 11 | -19.718 | -6.079 | -14.666 | 1.00 | 1.20 |
| ATOM | 87 | OG | SER | 11 | -20.246 | -5.067 | -16.365 | 1.00 | 1.39 |
| ATOM | 88 | HG | SER | 11 | -19.821 | -4.495 | -17.008 | 1.00 | 1.92 |
| ATOM | 89 | C | SER | 11 | -17.893 | -5.335 | -17.379 | 1.00 | 0.47 |
| ATOM | 90 | O | SER | 11 | -18.785 | -5.528 | -18.181 | 1.00 | 0.60 |
| ATOM | 91 | N | LYS | 12 | -16.808 | -4.692 | -17.715 | 1.00 | 0.42 |
| ATOM | 92 | HN | LYS | 12 | -16.101 | -4.543 | -17.053 | 1.00 | 0.51 |
| ATOM | 93 | CA | LYS | 12 | -16.646 | -4.178 | -19.107 | 1.00 | 0.41 |
| ATOM | 94 | HA | LYS | 12 | -17.243 | -4.775 | -19.781 | 1.00 | 0.47 |
| ATOM | 95 | CB | LYS | 12 | -17.116 | -2.722 | -19.167 | 1.00 | 0.43 |
| ATOM | 96 | HB1 | LYS | 12 | -18.168 | -2.674 | -18.926 | 1.00 | 0.50 |
| ATOM | 97 | HB2 | LYS | 12 | -16.957 | -2.334 | -20.163 | 1.00 | 0.46 |
| ATOM | 98 | CG | LYS | 12 | -16.327 | -1.882 | -18.160 | 1.00 | 0.41 |
| ATOM | 99 | HG1 | LYS | 12 | -15.275 | -1.922 | -18.401 | 1.00 | 0.37 |
| ATOM | 100 | HG2 | LYS | 12 | -16.484 | -2.272 | -17.164 | 1.00 | 0.42 |
| ATOM | 101 | CD | LYS | 12 | -16.805 | -0.430 | -18.223 | 1.00 | 0.50 |
| ATOM | 102 | HD1 | LYS | 12 | -17.856 | -0.386 | -17.981 | 1.00 | 0.56 |
| ATOM | 103 | HD2 | LYS | 12 | -16.648 | -0.044 | -19.220 | 1.00 | 0.65 |
| ATOM | 104 | CE | LYS | 12 | -16.018 | 0.412 | -17.218 | 1.00 | 0.61 |
| ATOM | 105 | HE1 | LYS | 12 | -15.054 | 0.665 | -17.636 | 1.00 | 1.15 |
| ATOM | 106 | HE2 | LYS | 12 | -15.879 | -0.151 | -16.307 | 1.00 | 1.16 |
| ATOM | 107 | NZ | LYS | 12 | -16.773 | 1.661 | -16.920 | 1.00 | 1.39 |
| ATOM | 108 | HZ1 | LYS | 12 | -16.498 | 2.018 | -15.983 | 1.00 | 1.90 |
| ATOM | 109 | HZ2 | LYS | 12 | -17.794 | 1.458 | -16.927 | 1.00 | 1.87 |
| ATOM | 110 | HZ3 | LYS | 12 | -16.556 | 2.379 | -17.640 | 1.00 | 1.97 |
| ATOM | 111 | C | LYS | 12 | -15.175 | -4.269 | -19.521 | 1.00 | 0.36 |
| ATOM | 112 | O | LYS | 12 | -14.284 | -4.250 | -18.695 | 1.00 | 0.34 |
| ATOM | 113 | N | MET | 13 | -14.917 | -4.380 | -20.796 | 1.00 | 0.37 |
| ATOM | 114 | HN | MET | 13 | -15.652 | -4.402 | -21.443 | 1.00 | 0.40 |
| ATOM | 115 | CA | MET | 13 | -13.506 | -4.487 | -21.269 | 1.00 | 0.38 |
| ATOM | 116 | HA | MET | 13 | -12.910 | -4.964 | -20.506 | 1.00 | 0.39 |

6/75

| | | | | | | | | | |
|------|-----|------|-----|----|---------|--------|---------|------|------|
| ATOM | 117 | CB | MET | 13 | -13.469 | -5.332 | -22.543 | 1.00 | 0.46 |
| ATOM | 118 | HB1 | MET | 13 | -12.523 | -5.189 | -23.043 | 1.00 | 0.53 |
| ATOM | 119 | HB2 | MET | 13 | -14.273 | -5.031 | -23.199 | 1.00 | 0.42 |
| ATOM | 120 | CG | MET | 13 | -13.632 | -6.809 | -22.178 | 1.00 | 0.64 |
| ATOM | 121 | HG1 | MET | 13 | -12.857 | -7.097 | -21.483 | 1.00 | 1.26 |
| ATOM | 122 | HG2 | MET | 13 | -13.556 | -7.411 | -23.071 | 1.00 | 1.37 |
| ATOM | 123 | SD | MET | 13 | -15.252 | -7.067 | -21.414 | 1.00 | 1.22 |
| ATOM | 124 | CE | MET | 13 | -14.663 | -7.870 | -19.903 | 1.00 | 0.57 |
| ATOM | 125 | HE1 | MET | 13 | -14.020 | -7.189 | -19.362 | 1.00 | 1.16 |
| ATOM | 126 | HE2 | MET | 13 | -14.107 | -8.758 | -20.158 | 1.00 | 1.09 |
| ATOM | 127 | HE3 | MET | 13 | -15.508 | -8.141 | -19.286 | 1.00 | 1.20 |
| ATOM | 128 | C | MET | 13 | -12.936 | -3.095 | -21.560 | 1.00 | 0.32 |
| ATOM | 129 | O | MET | 13 | -11.793 | -2.957 | -21.948 | 1.00 | 0.35 |
| ATOM | 130 | N | ASN | 14 | -13.718 | -2.064 | -21.371 | 1.00 | 0.28 |
| ATOM | 131 | HN | ASN | 14 | -14.635 | -2.199 | -21.052 | 1.00 | 0.29 |
| ATOM | 132 | CA | ASN | 14 | -13.217 | -0.681 | -21.631 | 1.00 | 0.26 |
| ATOM | 133 | HA | ASN | 14 | -12.359 | -0.725 | -22.286 | 1.00 | 0.29 |
| ATOM | 134 | CB | ASN | 14 | -14.319 | 0.148 | -22.297 | 1.00 | 0.30 |
| ATOM | 135 | HB1 | ASN | 14 | -14.025 | 1.186 | -22.318 | 1.00 | 0.31 |
| ATOM | 136 | HB2 | ASN | 14 | -15.235 | 0.043 | -21.735 | 1.00 | 0.31 |
| ATOM | 137 | CG | ASN | 14 | -14.539 | -0.346 | -23.729 | 1.00 | 0.37 |
| ATOM | 138 | OD1 | ASN | 14 | -13.677 | -0.981 | -24.304 | 1.00 | 1.16 |
| ATOM | 139 | ND2 | ASN | 14 | -15.664 | -0.077 | -24.334 | 1.00 | 1.05 |
| ATOM | 140 | HD21 | ASN | 14 | -16.359 | 0.435 | -23.871 | 1.00 | 1.81 |
| ATOM | 141 | HD22 | ASN | 14 | -15.812 | -0.386 | -25.252 | 1.00 | 1.06 |
| ATOM | 142 | C | ASN | 14 | -12.813 | -0.024 | -20.309 | 1.00 | 0.22 |
| ATOM | 143 | O | ASN | 14 | -13.566 | -0.019 | -19.357 | 1.00 | 0.23 |
| ATOM | 144 | N | LEU | 15 | -11.630 | 0.533 | -20.247 | 1.00 | 0.21 |
| ATOM | 145 | HN | LEU | 15 | -11.042 | 0.517 | -21.031 | 1.00 | 0.24 |
| ATOM | 146 | CA | LEU | 15 | -11.171 | 1.194 | -18.987 | 1.00 | 0.18 |
| ATOM | 147 | HA | LEU | 15 | -12.025 | 1.447 | -18.379 | 1.00 | 0.19 |
| ATOM | 148 | CB | LEU | 15 | -10.250 | 0.243 | -18.210 | 1.00 | 0.18 |
| ATOM | 149 | HB1 | LEU | 15 | -9.812 | 0.769 | -17.375 | 1.00 | 0.19 |
| ATOM | 150 | HB2 | LEU | 15 | -9.463 | -0.102 | -18.865 | 1.00 | 0.21 |
| ATOM | 151 | CG | LEU | 15 | -11.046 | -0.964 | -17.696 | 1.00 | 0.19 |
| ATOM | 152 | HG | LEU | 15 | -11.547 | -1.442 | -18.525 | 1.00 | 0.20 |
| ATOM | 153 | CD1 | LEU | 15 | -10.086 | -1.961 | -17.044 | 1.00 | 0.20 |
| ATOM | 154 | HD11 | LEU | 15 | -9.726 | -1.556 | -16.110 | 1.00 | 0.98 |
| ATOM | 155 | HD12 | LEU | 15 | -9.251 | -2.141 | -17.704 | 1.00 | 1.04 |
| ATOM | 156 | HD13 | LEU | 15 | -10.604 | -2.890 | -16.857 | 1.00 | 1.07 |
| ATOM | 157 | CD2 | LEU | 15 | -12.083 | -0.513 | -16.658 | 1.00 | 0.21 |
| ATOM | 158 | HD21 | LEU | 15 | -12.114 | -1.228 | -15.850 | 1.00 | 1.07 |
| ATOM | 159 | HD22 | LEU | 15 | -13.055 | -0.456 | -17.122 | 1.00 | 1.00 |
| ATOM | 160 | HD23 | LEU | 15 | -11.814 | 0.457 | -16.268 | 1.00 | 1.04 |
| ATOM | 161 | C | LEU | 15 | -10.397 | 2.471 | -19.334 | 1.00 | 0.18 |
| ATOM | 162 | O | LEU | 15 | -9.785 | 2.570 | -20.380 | 1.00 | 0.20 |
| ATOM | 163 | N | THR | 16 | -10.425 | 3.447 | -18.460 | 1.00 | 0.18 |
| ATOM | 164 | HN | THR | 16 | -10.929 | 3.338 | -17.627 | 1.00 | 0.18 |
| ATOM | 165 | CA | THR | 16 | -9.699 | 4.729 | -18.722 | 1.00 | 0.19 |
| ATOM | 166 | HA | THR | 16 | -9.051 | 4.617 | -19.574 | 1.00 | 0.20 |
| ATOM | 167 | CB | THR | 16 | -10.716 | 5.839 | -18.996 | 1.00 | 0.22 |
| ATOM | 168 | HB | THR | 16 | -10.198 | 6.729 | -19.315 | 1.00 | 0.24 |
| ATOM | 169 | OG1 | THR | 16 | -11.445 | 6.112 | -17.808 | 1.00 | 0.23 |
| ATOM | 170 | HG1 | THR | 16 | -11.821 | 5.286 | -17.495 | 1.00 | 0.98 |
| ATOM | 171 | CG2 | THR | 16 | -11.680 | 5.393 | -20.096 | 1.00 | 0.26 |
| ATOM | 172 | HG21 | THR | 16 | -12.200 | 6.254 | -20.489 | 1.00 | 1.05 |
| ATOM | 173 | HG22 | THR | 16 | -12.396 | 4.696 | -19.686 | 1.00 | 1.02 |
| ATOM | 174 | HG23 | THR | 16 | -11.125 | 4.914 | -20.889 | 1.00 | 1.05 |
| ATOM | 175 | C | THR | 16 | -8.864 | 5.100 | -17.495 | 1.00 | 0.17 |
| ATOM | 176 | O | THR | 16 | -9.157 | 4.687 | -16.391 | 1.00 | 0.16 |
| ATOM | 177 | N | TYR | 17 | -7.826 | 5.878 | -17.675 | 1.00 | 0.18 |
| ATOM | 178 | HN | TYR | 17 | -7.603 | 6.202 | -18.574 | 1.00 | 0.19 |
| ATOM | 179 | CA | TYR | 17 | -6.981 | 6.268 | -16.507 | 1.00 | 0.17 |
| ATOM | 180 | HA | TYR | 17 | -7.585 | 6.233 | -15.615 | 1.00 | 0.17 |
| ATOM | 181 | CB | TYR | 17 | -5.814 | 5.288 | -16.362 | 1.00 | 0.19 |
| ATOM | 182 | HB1 | TYR | 17 | -6.194 | 4.278 | -16.347 | 1.00 | 0.19 |
| ATOM | 183 | HB2 | TYR | 17 | -5.292 | 5.488 | -15.438 | 1.00 | 0.20 |
| ATOM | 184 | CG | TYR | 17 | -4.857 | 5.445 | -17.520 | 1.00 | 0.22 |
| ATOM | 185 | CD1 | TYR | 17 | -5.037 | 4.685 | -18.682 | 1.00 | 0.26 |
| ATOM | 186 | HD1 | TYR | 17 | -5.867 | 3.998 | -18.755 | 1.00 | 0.27 |
| ATOM | 187 | CD2 | TYR | 17 | -3.782 | 6.336 | -17.426 | 1.00 | 0.25 |
| ATOM | 188 | HD2 | TYR | 17 | -3.643 | 6.923 | -16.530 | 1.00 | 0.26 |
| ATOM | 189 | CE1 | TYR | 17 | -4.143 | 4.817 | -19.751 | 1.00 | 0.31 |
| ATOM | 190 | HE1 | TYR | 17 | -4.282 | 4.231 | -20.647 | 1.00 | 0.36 |
| ATOM | 191 | CE2 | TYR | 17 | -2.888 | 6.470 | -18.496 | 1.00 | 0.30 |
| ATOM | 192 | HE2 | TYR | 17 | -2.059 | 7.158 | -18.424 | 1.00 | 0.35 |
| ATOM | 193 | CZ | TYR | 17 | -3.068 | 5.710 | -19.658 | 1.00 | 0.32 |

7/75

| | | | | | | | | | |
|------|-----|------|-----|----|--------|--------|---------|------|------|
| ATOM | 194 | OH | TYR | 17 | -2.186 | 5.839 | -20.711 | 1.00 | 0.39 |
| ATOM | 195 | HH | TYR | 17 | -1.696 | 5.016 | -20.790 | 1.00 | 0.85 |
| ATOM | 196 | C | TYR | 17 | -6.448 | 7.692 | -16.690 | 1.00 | 0.19 |
| ATOM | 197 | O | TYR | 17 | -6.414 | 8.220 | -17.784 | 1.00 | 0.21 |
| ATOM | 198 | N | ARG | 18 | -6.044 | 8.320 | -15.616 | 1.00 | 0.19 |
| ATOM | 199 | HN | ARG | 18 | -6.089 | 7.874 | -14.747 | 1.00 | 0.19 |
| ATOM | 200 | CA | ARG | 18 | -5.523 | 9.714 | -15.712 | 1.00 | 0.22 |
| ATOM | 201 | HA | ARG | 18 | -5.131 | 9.877 | -16.704 | 1.00 | 0.24 |
| ATOM | 202 | CB | ARG | 18 | -6.674 | 10.691 | -15.447 | 1.00 | 0.27 |
| ATOM | 203 | HB1 | ARG | 18 | -6.978 | 10.613 | -14.412 | 1.00 | 0.31 |
| ATOM | 204 | HB2 | ARG | 18 | -7.507 | 10.442 | -16.083 | 1.00 | 0.30 |
| ATOM | 205 | CG | ARG | 18 | -6.229 | 12.127 | -15.733 | 1.00 | 0.35 |
| ATOM | 206 | HG1 | ARG | 18 | -5.504 | 12.137 | -16.531 | 1.00 | 0.93 |
| ATOM | 207 | HG2 | ARG | 18 | -5.790 | 12.549 | -14.843 | 1.00 | 0.85 |
| ATOM | 208 | CD | ARG | 18 | -7.447 | 12.946 | -16.149 | 1.00 | 0.81 |
| ATOM | 209 | HD1 | ARG | 18 | -8.216 | 12.867 | -15.378 | 1.00 | 1.29 |
| ATOM | 210 | HD2 | ARG | 18 | -7.838 | 12.561 | -17.068 | 1.00 | 1.63 |
| ATOM | 211 | NE | ARG | 18 | -7.030 | 14.362 | -16.406 | 1.00 | 1.52 |
| ATOM | 212 | HE | ARG | 18 | -7.071 | 14.711 | -17.318 | 1.00 | 2.11 |
| ATOM | 213 | CZ | ARG | 18 | -6.561 | 15.119 | -15.456 | 1.00 | 2.24 |
| ATOM | 214 | NH1 | ARG | 18 | -6.119 | 16.314 | -15.736 | 1.00 | 3.18 |
| ATOM | 215 | HH11 | ARG | 18 | -6.142 | 16.647 | -16.679 | 1.00 | 3.48 |
| ATOM | 216 | HH12 | ARG | 18 | -5.760 | 16.898 | -15.009 | 1.00 | 3.84 |
| ATOM | 217 | NH2 | ARG | 18 | -6.564 | 14.700 | -14.220 | 1.00 | 2.63 |
| ATOM | 218 | HH21 | ARG | 18 | -6.928 | 13.795 | -14.000 | 1.00 | 2.44 |
| ATOM | 219 | HH22 | ARG | 18 | -6.205 | 15.285 | -13.493 | 1.00 | 3.49 |
| ATOM | 220 | C | ARG | 18 | -4.413 | 9.931 | -14.676 | 1.00 | 0.21 |
| ATOM | 221 | O | ARG | 18 | -4.550 | 9.576 | -13.522 | 1.00 | 0.23 |
| ATOM | 222 | N | ILE | 19 | -3.314 | 10.514 | -15.079 | 1.00 | 0.21 |
| ATOM | 223 | HN | ILE | 19 | -3.223 | 10.794 | -16.014 | 1.00 | 0.22 |
| ATOM | 224 | CA | ILE | 19 | -2.196 | 10.755 | -14.118 | 1.00 | 0.23 |
| ATOM | 225 | HA | ILE | 19 | -2.200 | 9.985 | -13.360 | 1.00 | 0.25 |
| ATOM | 226 | CB | ILE | 19 | -0.864 | 10.721 | -14.875 | 1.00 | 0.25 |
| ATOM | 227 | HB | ILE | 19 | -0.862 | 11.491 | -15.633 | 1.00 | 0.25 |
| ATOM | 228 | CG1 | ILE | 19 | -0.702 | 9.341 | -15.531 | 1.00 | 0.29 |
| ATOM | 229 | HG11 | ILE | 19 | -1.607 | 9.092 | -16.065 | 1.00 | 0.82 |
| ATOM | 230 | HG12 | ILE | 19 | -0.525 | 8.601 | -14.765 | 1.00 | 0.97 |
| ATOM | 231 | CG2 | ILE | 19 | 0.291 | 10.962 | -13.893 | 1.00 | 0.29 |
| ATOM | 232 | HG21 | ILE | 19 | 1.231 | 10.914 | -14.420 | 1.00 | 1.08 |
| ATOM | 233 | HG22 | ILE | 19 | 0.272 | 10.206 | -13.123 | 1.00 | 1.09 |
| ATOM | 234 | HG23 | ILE | 19 | 0.187 | 11.937 | -13.440 | 1.00 | 1.00 |
| ATOM | 235 | CD1 | ILE | 19 | 0.477 | 9.345 | -16.512 | 1.00 | 0.93 |
| ATOM | 236 | HD11 | ILE | 19 | 1.402 | 9.216 | -15.970 | 1.00 | 1.59 |
| ATOM | 237 | HD12 | ILE | 19 | 0.501 | 10.280 | -17.050 | 1.00 | 1.50 |
| ATOM | 238 | HD13 | ILE | 19 | 0.360 | 8.533 | -17.214 | 1.00 | 1.55 |
| ATOM | 239 | C | ILE | 19 | -2.381 | 12.126 | -13.454 | 1.00 | 0.23 |
| ATOM | 240 | O | ILE | 19 | -2.355 | 13.150 | -14.108 | 1.00 | 0.23 |
| ATOM | 241 | N | VAL | 20 | -2.563 | 12.152 | -12.161 | 1.00 | 0.25 |
| ATOM | 242 | HN | VAL | 20 | -2.578 | 11.314 | -11.653 | 1.00 | 0.27 |
| ATOM | 243 | CA | VAL | 20 | -2.746 | 13.454 | -11.454 | 1.00 | 0.27 |
| ATOM | 244 | HA | VAL | 20 | -3.496 | 14.035 | -11.970 | 1.00 | 0.27 |
| ATOM | 245 | CB | VAL | 20 | -3.202 | 13.205 | -10.015 | 1.00 | 0.31 |
| ATOM | 246 | HB | VAL | 20 | -2.522 | 12.517 | -9.534 | 1.00 | 0.32 |
| ATOM | 247 | CG1 | VAL | 20 | -3.216 | 14.529 | -9.247 | 1.00 | 0.33 |
| ATOM | 248 | HG11 | VAL | 20 | -3.607 | 15.310 | -9.883 | 1.00 | 0.97 |
| ATOM | 249 | HG12 | VAL | 20 | -2.211 | 14.782 | -8.944 | 1.00 | 1.08 |
| ATOM | 250 | HG13 | VAL | 20 | -3.842 | 14.432 | -8.372 | 1.00 | 1.10 |
| ATOM | 251 | CG2 | VAL | 20 | -4.612 | 12.611 | -10.028 | 1.00 | 0.33 |
| ATOM | 252 | HG21 | VAL | 20 | -5.296 | 13.317 | -10.476 | 1.00 | 1.05 |
| ATOM | 253 | HG22 | VAL | 20 | -4.924 | 12.401 | -9.016 | 1.00 | 1.03 |
| ATOM | 254 | HG23 | VAL | 20 | -4.612 | 11.697 | -10.602 | 1.00 | 1.11 |
| ATOM | 255 | C | VAL | 20 | -1.424 | 14.231 | -11.451 | 1.00 | 0.27 |
| ATOM | 256 | O | VAL | 20 | -1.403 | 15.435 | -11.611 | 1.00 | 0.26 |
| ATOM | 257 | N | ASN | 21 | -0.321 | 13.555 | -11.259 | 1.00 | 0.28 |
| ATOM | 258 | HN | ASN | 21 | -0.357 | 12.585 | -11.124 | 1.00 | 0.30 |
| ATOM | 259 | CA | ASN | 21 | 0.992 | 14.265 | -11.235 | 1.00 | 0.29 |
| ATOM | 260 | HA | ASN | 21 | 0.973 | 15.076 | -11.949 | 1.00 | 0.26 |
| ATOM | 261 | CB | ASN | 21 | 1.235 | 14.829 | -9.834 | 1.00 | 0.33 |
| ATOM | 262 | HB1 | ASN | 21 | 0.544 | 15.637 | -9.646 | 1.00 | 0.33 |
| ATOM | 263 | HB2 | ASN | 21 | 2.249 | 15.199 | -9.766 | 1.00 | 0.35 |
| ATOM | 264 | CG | ASN | 21 | 1.022 | 13.727 | -8.795 | 1.00 | 0.40 |
| ATOM | 265 | OD1 | ASN | 21 | 0.459 | 12.694 | -9.097 | 1.00 | 1.01 |
| ATOM | 266 | ND2 | ASN | 21 | 1.445 | 13.908 | -7.574 | 1.00 | 0.88 |
| ATOM | 267 | HD21 | ASN | 21 | 1.895 | 14.743 | -7.330 | 1.00 | 1.50 |
| ATOM | 268 | HD22 | ASN | 21 | 1.312 | 13.208 | -6.901 | 1.00 | 0.88 |
| ATOM | 269 | C | ASN | 21 | 2.116 | 13.291 | -11.606 | 1.00 | 0.34 |
| ATOM | 270 | O | ASN | 21 | 1.929 | 12.090 | -11.619 | 1.00 | 0.37 |

8/75

| | | | | | | | | | |
|------|-----|------|-----|----|--------|--------|---------|------|------|
| ATOM | 271 | N | TYR | 22 | 3.274 | 13.810 | -11.933 | 1.00 | 0.38 |
| ATOM | 272 | HN | TYR | 22 | 3.387 | 14.783 | -11.932 | 1.00 | 0.38 |
| ATOM | 273 | CA | TYR | 22 | 4.417 | 12.935 | -12.340 | 1.00 | 0.46 |
| ATOM | 274 | HA | TYR | 22 | 4.067 | 11.929 | -12.509 | 1.00 | 0.45 |
| ATOM | 275 | CB | TYR | 22 | 5.028 | 13.481 | -13.630 | 1.00 | 0.49 |
| ATOM | 276 | HB1 | TYR | 22 | 5.845 | 12.846 | -13.938 | 1.00 | 0.56 |
| ATOM | 277 | HB2 | TYR | 22 | 5.397 | 14.482 | -13.457 | 1.00 | 0.53 |
| ATOM | 278 | CG | TYR | 22 | 3.981 | 13.513 | -14.714 | 1.00 | 0.43 |
| ATOM | 279 | CD1 | TYR | 22 | 3.684 | 12.352 | -15.436 | 1.00 | 0.38 |
| ATOM | 280 | HD1 | TYR | 22 | 4.199 | 11.430 | -15.212 | 1.00 | 0.39 |
| ATOM | 281 | CD2 | TYR | 22 | 3.313 | 14.708 | -15.003 | 1.00 | 0.46 |
| ATOM | 282 | HD2 | TYR | 22 | 3.543 | 15.603 | -14.445 | 1.00 | 0.51 |
| ATOM | 283 | CE1 | TYR | 22 | 2.718 | 12.386 | -16.447 | 1.00 | 0.36 |
| ATOM | 284 | HE1 | TYR | 22 | 2.490 | 11.491 | -17.004 | 1.00 | 0.36 |
| ATOM | 285 | CE2 | TYR | 22 | 2.345 | 14.742 | -16.013 | 1.00 | 0.44 |
| ATOM | 286 | HE2 | TYR | 22 | 1.828 | 15.663 | -16.235 | 1.00 | 0.49 |
| ATOM | 287 | CZ | TYR | 22 | 2.048 | 13.581 | -16.735 | 1.00 | 0.39 |
| ATOM | 288 | OH | TYR | 22 | 1.095 | 13.615 | -17.733 | 1.00 | 0.43 |
| ATOM | 289 | HH | TYR | 22 | 1.173 | 14.457 | -18.187 | 1.00 | 0.92 |
| ATOM | 290 | C | TYR | 22 | 5.499 | 12.923 | -11.258 | 1.00 | 0.56 |
| ATOM | 291 | O | TYR | 22 | 6.554 | 12.378 | -11.470 | 1.00 | 1.38 |
| ATOM | 292 | N | THR | 23 | 5.240 | 13.544 | -10.130 | 1.00 | 0.47 |
| ATOM | 293 | HN | THR | 23 | 4.372 | 13.987 | -10.023 | 1.00 | 1.08 |
| ATOM | 294 | CA | THR | 23 | 6.237 | 13.623 | -9.004 | 1.00 | 0.46 |
| ATOM | 295 | HA | THR | 23 | 5.848 | 14.338 | -8.304 | 1.00 | 0.48 |
| ATOM | 296 | CB | THR | 23 | 6.361 | 12.265 | -8.273 | 1.00 | 0.62 |
| ATOM | 297 | HB | THR | 23 | 5.383 | 11.969 | -7.921 | 1.00 | 0.68 |
| ATOM | 298 | OG1 | THR | 23 | 7.223 | 12.420 | -7.156 | 1.00 | 0.86 |
| ATOM | 299 | HG1 | THR | 23 | 7.941 | 11.788 | -7.244 | 1.00 | 1.28 |
| ATOM | 300 | CG2 | THR | 23 | 6.916 | 11.159 | -9.181 | 1.00 | 0.59 |
| ATOM | 301 | HG21 | THR | 23 | 7.753 | 11.533 | -9.748 | 1.00 | 1.08 |
| ATOM | 302 | HG22 | THR | 23 | 6.141 | 10.816 | -9.850 | 1.00 | 1.16 |
| ATOM | 303 | HG23 | THR | 23 | 7.245 | 10.332 | -8.570 | 1.00 | 1.22 |
| ATOM | 304 | C | THR | 23 | 7.623 | 14.115 | -9.523 | 1.00 | 0.40 |
| ATOM | 305 | O | THR | 23 | 8.077 | 13.699 | -10.565 | 1.00 | 0.45 |
| ATOM | 306 | N | PRO | 24 | 8.302 | 15.016 | -8.823 | 1.00 | 0.42 |
| ATOM | 307 | CA | PRO | 24 | 9.625 | 15.520 | -9.311 | 1.00 | 0.42 |
| ATOM | 308 | HA | PRO | 24 | 9.534 | 15.918 | -10.307 | 1.00 | 0.46 |
| ATOM | 309 | CB | PRO | 24 | 9.924 | 16.655 | -8.335 | 1.00 | 0.50 |
| ATOM | 310 | HB1 | PRO | 24 | 9.743 | 17.605 | -8.815 | 1.00 | 0.57 |
| ATOM | 311 | HB2 | PRO | 24 | 10.955 | 16.598 | -8.014 | 1.00 | 0.49 |
| ATOM | 312 | CG | PRO | 24 | 8.995 | 16.507 | -7.129 | 1.00 | 0.66 |
| ATOM | 313 | HG1 | PRO | 24 | 8.613 | 17.475 | -6.842 | 1.00 | 0.84 |
| ATOM | 314 | HG2 | PRO | 24 | 9.537 | 16.069 | -6.303 | 1.00 | 0.76 |
| ATOM | 315 | CD | PRO | 24 | 7.832 | 15.598 | -7.529 | 1.00 | 0.56 |
| ATOM | 316 | HD2 | PRO | 24 | 7.675 | 14.826 | -6.786 | 1.00 | 0.62 |
| ATOM | 317 | HD1 | PRO | 24 | 6.940 | 16.183 | -7.680 | 1.00 | 0.61 |
| ATOM | 318 | C | PRO | 24 | 10.743 | 14.470 | -9.253 | 1.00 | 0.40 |
| ATOM | 319 | O | PRO | 24 | 11.835 | 14.692 | -9.737 | 1.00 | 0.40 |
| ATOM | 320 | N | ASP | 25 | 10.490 | 13.337 | -8.662 | 1.00 | 0.44 |
| ATOM | 321 | HN | ASP | 25 | 9.608 | 13.172 | -8.270 | 1.00 | 0.48 |
| ATOM | 322 | CA | ASP | 25 | 11.554 | 12.295 | -8.577 | 1.00 | 0.48 |
| ATOM | 323 | HA | ASP | 25 | 12.393 | 12.695 | -8.025 | 1.00 | 0.51 |
| ATOM | 324 | CB | ASP | 25 | 11.016 | 11.062 | -7.847 | 1.00 | 0.57 |
| ATOM | 325 | HB1 | ASP | 25 | 11.719 | 10.249 | -7.945 | 1.00 | 0.61 |
| ATOM | 326 | HB2 | ASP | 25 | 10.068 | 10.773 | -8.276 | 1.00 | 0.56 |
| ATOM | 327 | CG | ASP | 25 | 10.827 | 11.394 | -6.364 | 1.00 | 0.67 |
| ATOM | 328 | OD1 | ASP | 25 | 10.079 | 10.689 | -5.709 | 1.00 | 1.23 |
| ATOM | 329 | OD2 | ASP | 25 | 11.437 | 12.348 | -5.908 | 1.00 | 1.34 |
| ATOM | 330 | C | ASP | 25 | 12.025 | 11.916 | -9.985 | 1.00 | 0.45 |
| ATOM | 331 | O | ASP | 25 | 13.179 | 11.597 | -10.191 | 1.00 | 0.55 |
| ATOM | 332 | N | MET | 26 | 11.146 | 11.948 | -10.955 | 1.00 | 0.40 |
| ATOM | 333 | HN | MET | 26 | 10.220 | 12.209 | -10.767 | 1.00 | 0.41 |
| ATOM | 334 | CA | MET | 26 | 11.553 | 11.590 | -12.348 | 1.00 | 0.42 |
| ATOM | 335 | HA | MET | 26 | 12.624 | 11.686 | -12.447 | 1.00 | 0.49 |
| ATOM | 336 | CB | MET | 26 | 11.144 | 10.149 | -12.656 | 1.00 | 0.53 |
| ATOM | 337 | HB1 | MET | 26 | 11.282 | 9.954 | -13.709 | 1.00 | 0.55 |
| ATOM | 338 | HB2 | MET | 26 | 10.105 | 10.006 | -12.397 | 1.00 | 0.51 |
| ATOM | 339 | CG | MET | 26 | 12.011 | 9.186 | -11.846 | 1.00 | 0.71 |
| ATOM | 340 | HG1 | MET | 26 | 11.783 | 9.288 | -10.796 | 1.00 | 0.73 |
| ATOM | 341 | HG2 | MET | 26 | 13.053 | 9.419 | -12.009 | 1.00 | 0.77 |
| ATOM | 342 | SD | MET | 26 | 11.683 | 7.485 | -12.380 | 1.00 | 0.89 |
| ATOM | 343 | CE | MET | 26 | 10.000 | 7.330 | -11.728 | 1.00 | 0.59 |
| ATOM | 344 | HE1 | MET | 26 | 9.292 | 7.456 | -12.534 | 1.00 | 1.25 |
| ATOM | 345 | HE2 | MET | 26 | 9.825 | 8.084 | -10.979 | 1.00 | 1.23 |
| ATOM | 346 | HE3 | MET | 26 | 9.877 | 6.352 | -11.285 | 1.00 | 1.23 |
| ATOM | 347 | C | MET | 26 | 10.872 | 12.530 | -13.344 | 1.00 | 0.34 |

9/75

| | | | | | | | | | |
|------|-----|------|-----|----|--------|--------|---------|------|------|
| ATOM | 348 | O | MET | 26 | 9.897 | 13.184 | -13.031 | 1.00 | 0.32 |
| ATOM | 349 | N | THR | 27 | 11.385 | 12.604 | -14.544 | 1.00 | 0.33 |
| ATOM | 350 | HN | THR | 27 | 12.174 | 12.070 | -14.773 | 1.00 | 0.38 |
| ATOM | 351 | CA | THR | 27 | 10.775 | 13.504 | -15.562 | 1.00 | 0.32 |
| ATOM | 352 | HA | THR | 27 | 10.618 | 14.483 | -15.133 | 1.00 | 0.35 |
| ATOM | 353 | CB | THR | 27 | 11.711 | 13.616 | -16.768 | 1.00 | 0.39 |
| ATOM | 354 | HB | THR | 27 | 11.295 | 14.308 | -17.484 | 1.00 | 0.42 |
| ATOM | 355 | OG1 | THR | 27 | 11.852 | 12.338 | -17.371 | 1.00 | 0.37 |
| ATOM | 356 | HG1 | THR | 27 | 12.765 | 12.242 | -17.653 | 1.00 | 0.94 |
| ATOM | 357 | CG2 | THR | 27 | 13.080 | 14.121 | -16.313 | 1.00 | 0.51 |
| ATOM | 358 | HG21 | THR | 27 | 13.602 | 14.553 | -17.154 | 1.00 | 1.14 |
| ATOM | 359 | HG22 | THR | 27 | 13.655 | 13.297 | -15.918 | 1.00 | 1.11 |
| ATOM | 360 | HG23 | THR | 27 | 12.951 | 14.871 | -15.546 | 1.00 | 1.12 |
| ATOM | 361 | C | THR | 27 | 9.436 | 12.921 | -16.013 | 1.00 | 0.27 |
| ATOM | 362 | O | THR | 27 | 9.177 | 11.743 | -15.864 | 1.00 | 0.24 |
| ATOM | 363 | N | HIS | 28 | 8.580 | 13.740 | -16.554 | 1.00 | 0.32 |
| ATOM | 364 | HN | HIS | 28 | 8.807 | 14.688 | -16.657 | 1.00 | 0.37 |
| ATOM | 365 | CA | HIS | 28 | 7.253 | 13.241 | -17.004 | 1.00 | 0.34 |
| ATOM | 366 | HA | HIS | 28 | 6.715 | 12.833 | -16.161 | 1.00 | 0.36 |
| ATOM | 367 | CB | HIS | 28 | 6.457 | 14.403 | -17.601 | 1.00 | 0.46 |
| ATOM | 368 | HB1 | HIS | 28 | 5.428 | 14.104 | -17.736 | 1.00 | 0.71 |
| ATOM | 369 | HB2 | HIS | 28 | 6.880 | 14.676 | -18.557 | 1.00 | 0.88 |
| ATOM | 370 | CG | HIS | 28 | 6.516 | 15.583 | -16.669 | 1.00 | 0.73 |
| ATOM | 371 | ND1 | HIS | 28 | 6.056 | 16.838 | -17.036 | 1.00 | 1.66 |
| ATOM | 372 | HD1 | HIS | 28 | 5.659 | 17.080 | -17.898 | 1.00 | 2.30 |
| ATOM | 373 | CD2 | HIS | 28 | 6.987 | 15.716 | -15.387 | 1.00 | 1.33 |
| ATOM | 374 | HD2 | HIS | 28 | 7.423 | 14.922 | -14.798 | 1.00 | 2.01 |
| ATOM | 375 | CE1 | HIS | 28 | 6.258 | 17.664 | -15.993 | 1.00 | 1.95 |
| ATOM | 376 | HE1 | HIS | 28 | 5.993 | 18.711 | -15.990 | 1.00 | 2.70 |
| ATOM | 377 | NE2 | HIS | 28 | 6.823 | 17.031 | -14.962 | 1.00 | 1.71 |
| ATOM | 378 | C | HIS | 28 | 7.436 | 12.156 | -18.069 | 1.00 | 0.30 |
| ATOM | 379 | O | HIS | 28 | 6.737 | 11.164 | -18.082 | 1.00 | 0.30 |
| ATOM | 380 | N | SER | 29 | 8.362 | 12.338 | -18.970 | 1.00 | 0.31 |
| ATOM | 381 | HN | SER | 29 | 8.912 | 13.149 | -18.952 | 1.00 | 0.34 |
| ATOM | 382 | CA | SER | 29 | 8.567 | 11.319 | -20.039 | 1.00 | 0.32 |
| ATOM | 383 | HA | SER | 29 | 7.660 | 11.217 | -20.615 | 1.00 | 0.35 |
| ATOM | 384 | CB | SER | 29 | 9.699 | 11.775 | -20.959 | 1.00 | 0.38 |
| ATOM | 385 | HB1 | SER | 29 | 9.973 | 10.963 | -21.621 | 1.00 | 0.39 |
| ATOM | 386 | HB2 | SER | 29 | 10.555 | 12.056 | -20.368 | 1.00 | 0.37 |
| ATOM | 387 | OG | SER | 29 | 9.265 | 12.896 | -21.717 | 1.00 | 0.45 |
| ATOM | 388 | HG | SER | 29 | 9.157 | 12.614 | -22.628 | 1.00 | 0.96 |
| ATOM | 389 | C | SER | 29 | 8.931 | 9.964 | -19.424 | 1.00 | 0.26 |
| ATOM | 390 | O | SER | 29 | 8.479 | 8.930 | -19.876 | 1.00 | 0.26 |
| ATOM | 391 | N | GLU | 30 | 9.747 | 9.954 | -18.405 | 1.00 | 0.24 |
| ATOM | 392 | HN | GLU | 30 | 10.107 | 10.796 | -18.056 | 1.00 | 0.25 |
| ATOM | 393 | CA | GLU | 30 | 10.137 | 8.657 | -17.779 | 1.00 | 0.22 |
| ATOM | 394 | HA | GLU | 30 | 10.484 | 7.978 | -18.542 | 1.00 | 0.25 |
| ATOM | 395 | CB | GLU | 30 | 11.260 | 8.899 | -16.769 | 1.00 | 0.23 |
| ATOM | 396 | HB1 | GLU | 30 | 11.424 | 8.002 | -16.191 | 1.00 | 0.24 |
| ATOM | 397 | HB2 | GLU | 30 | 10.980 | 9.707 | -16.108 | 1.00 | 0.22 |
| ATOM | 398 | CG | GLU | 30 | 12.547 | 9.268 | -17.510 | 1.00 | 0.29 |
| ATOM | 399 | HG1 | GLU | 30 | 12.386 | 10.165 | -18.086 | 1.00 | 0.67 |
| ATOM | 400 | HG2 | GLU | 30 | 12.826 | 8.460 | -18.171 | 1.00 | 0.68 |
| ATOM | 401 | CD | GLU | 30 | 13.666 | 9.509 | -16.495 | 1.00 | 0.84 |
| ATOM | 402 | OE1 | GLU | 30 | 13.436 | 9.266 | -15.321 | 1.00 | 1.49 |
| ATOM | 403 | OE2 | GLU | 30 | 14.731 | 9.936 | -16.908 | 1.00 | 1.59 |
| ATOM | 404 | C | GLU | 30 | 8.935 | 8.046 | -17.051 | 1.00 | 0.17 |
| ATOM | 405 | O | GLU | 30 | 8.715 | 6.849 | -17.082 | 1.00 | 0.19 |
| ATOM | 406 | N | VAL | 31 | 8.163 | 8.861 | -16.387 | 1.00 | 0.16 |
| ATOM | 407 | HN | VAL | 31 | 8.366 | 9.819 | -16.371 | 1.00 | 0.17 |
| ATOM | 408 | CA | VAL | 31 | 6.983 | 8.341 | -15.640 | 1.00 | 0.16 |
| ATOM | 409 | HA | VAL | 31 | 7.292 | 7.527 | -14.999 | 1.00 | 0.17 |
| ATOM | 410 | CB | VAL | 31 | 6.402 | 9.464 | -14.782 | 1.00 | 0.20 |
| ATOM | 411 | HB | VAL | 31 | 6.261 | 10.344 | -15.392 | 1.00 | 0.22 |
| ATOM | 412 | CG1 | VAL | 31 | 5.058 | 9.021 | -14.208 | 1.00 | 0.23 |
| ATOM | 413 | HG11 | VAL | 31 | 5.135 | 8.000 | -13.867 | 1.00 | 0.97 |
| ATOM | 414 | HG12 | VAL | 31 | 4.298 | 9.090 | -14.973 | 1.00 | 1.07 |
| ATOM | 415 | HG13 | VAL | 31 | 4.793 | 9.659 | -13.378 | 1.00 | 1.07 |
| ATOM | 416 | CG2 | VAL | 31 | 7.364 | 9.785 | -13.636 | 1.00 | 0.24 |
| ATOM | 417 | HG21 | VAL | 31 | 7.528 | 8.897 | -13.045 | 1.00 | 1.05 |
| ATOM | 418 | HG22 | VAL | 31 | 6.936 | 10.557 | -13.013 | 1.00 | 1.03 |
| ATOM | 419 | HG23 | VAL | 31 | 8.304 | 10.129 | -14.040 | 1.00 | 0.99 |
| ATOM | 420 | C | VAL | 31 | 5.911 | 7.844 | -16.617 | 1.00 | 0.16 |
| ATOM | 421 | O | VAL | 31 | 5.293 | 6.817 | -16.406 | 1.00 | 0.17 |
| ATOM | 422 | N | GLU | 32 | 5.672 | 8.571 | -17.677 | 1.00 | 0.18 |
| ATOM | 423 | HN | GLU | 32 | 6.172 | 9.401 | -17.824 | 1.00 | 0.19 |
| ATOM | 424 | CA | GLU | 32 | 4.626 | 8.146 | -18.652 | 1.00 | 0.21 |

10/75

| | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|---------|------|------|
| ATOM | 425 | HA | GLU | 32 | 3.673 | 8.092 | -18.147 | 1.00 | 0.24 |
| ATOM | 426 | CB | GLU | 32 | 4.533 | 9.170 | -19.787 | 1.00 | 0.27 |
| ATOM | 427 | HB1 | GLU | 32 | 3.922 | 8.772 | -20.582 | 1.00 | 0.31 |
| ATOM | 428 | HB2 | GLU | 32 | 5.524 | 9.379 | -20.164 | 1.00 | 0.28 |
| ATOM | 429 | CG | GLU | 32 | 3.904 | 10.463 | -19.262 | 1.00 | 0.29 |
| ATOM | 430 | HG1 | GLU | 32 | 4.456 | 10.812 | -18.405 | 1.00 | 0.48 |
| ATOM | 431 | HG2 | GLU | 32 | 2.879 | 10.272 | -18.977 | 1.00 | 0.52 |
| ATOM | 432 | CD | GLU | 32 | 3.937 | 11.529 | -20.359 | 1.00 | 0.70 |
| ATOM | 433 | OE1 | GLU | 32 | 4.969 | 12.161 | -20.513 | 1.00 | 1.37 |
| ATOM | 434 | OE2 | GLU | 32 | 2.929 | 11.696 | -21.026 | 1.00 | 1.45 |
| ATOM | 435 | C | GLU | 32 | 4.962 | 6.773 | -19.235 | 1.00 | 0.20 |
| ATOM | 436 | O | GLU | 32 | 4.126 | 5.893 | -19.280 | 1.00 | 0.20 |
| ATOM | 437 | N | LYS | 33 | 6.168 | 6.575 | -19.689 | 1.00 | 0.20 |
| ATOM | 438 | HN | LYS | 33 | 6.835 | 7.293 | -19.654 | 1.00 | 0.21 |
| ATOM | 439 | CA | LYS | 33 | 6.518 | 5.249 | -20.269 | 1.00 | 0.21 |
| ATOM | 440 | HA | LYS | 33 | 5.825 | 5.029 | -21.068 | 1.00 | 0.24 |
| ATOM | 441 | CB | LYS | 33 | 7.940 | 5.281 | -20.843 | 1.00 | 0.26 |
| ATOM | 442 | HB1 | LYS | 33 | 7.987 | 6.024 | -21.624 | 1.00 | 0.31 |
| ATOM | 443 | HB2 | LYS | 33 | 8.179 | 4.312 | -21.257 | 1.00 | 0.31 |
| ATOM | 444 | CG | LYS | 33 | 8.954 | 5.631 | -19.748 | 1.00 | 0.26 |
| ATOM | 445 | HG1 | LYS | 33 | 8.823 | 4.970 | -18.906 | 1.00 | 0.40 |
| ATOM | 446 | HG2 | LYS | 33 | 8.799 | 6.648 | -19.430 | 1.00 | 0.42 |
| ATOM | 447 | CD | LYS | 33 | 10.380 | 5.469 | -20.291 | 1.00 | 0.48 |
| ATOM | 448 | HD1 | LYS | 33 | 10.466 | 4.517 | -20.793 | 1.00 | 0.74 |
| ATOM | 449 | HD2 | LYS | 33 | 11.080 | 5.505 | -19.469 | 1.00 | 1.11 |
| ATOM | 450 | CE | LYS | 33 | 10.705 | 6.593 | -21.282 | 1.00 | 0.92 |
| ATOM | 451 | HE1 | LYS | 33 | 10.398 | 7.543 | -20.868 | 1.00 | 1.52 |
| ATOM | 452 | HE2 | LYS | 33 | 10.184 | 6.419 | -22.211 | 1.00 | 1.19 |
| ATOM | 453 | NZ | LYS | 33 | 12.172 | 6.614 | -21.538 | 1.00 | 1.60 |
| ATOM | 454 | HZ1 | LYS | 33 | 12.668 | 6.957 | -20.692 | 1.00 | 1.99 |
| ATOM | 455 | HZ2 | LYS | 33 | 12.374 | 7.247 | -22.340 | 1.00 | 2.14 |
| ATOM | 456 | HZ3 | LYS | 33 | 12.498 | 5.653 | -21.763 | 1.00 | 2.03 |
| ATOM | 457 | C | LYS | 33 | 6.399 | 4.158 | -19.202 | 1.00 | 0.19 |
| ATOM | 458 | O | LYS | 33 | 6.054 | 3.035 | -19.495 | 1.00 | 0.20 |
| ATOM | 459 | N | ALA | 34 | 6.682 | 4.471 | -17.966 | 1.00 | 0.17 |
| ATOM | 460 | HN | ALA | 34 | 6.965 | 5.383 | -17.740 | 1.00 | 0.18 |
| ATOM | 461 | CA | ALA | 34 | 6.589 | 3.428 | -16.904 | 1.00 | 0.16 |
| ATOM | 462 | HA | ALA | 34 | 7.276 | 2.625 | -17.128 | 1.00 | 0.18 |
| ATOM | 463 | CB | ALA | 34 | 6.952 | 4.043 | -15.551 | 1.00 | 0.16 |
| ATOM | 464 | HB1 | ALA | 34 | 6.483 | 3.476 | -14.761 | 1.00 | 1.02 |
| ATOM | 465 | HB2 | ALA | 34 | 6.604 | 5.065 | -15.516 | 1.00 | 0.98 |
| ATOM | 466 | HB3 | ALA | 34 | 8.024 | 4.022 | -15.423 | 1.00 | 1.02 |
| ATOM | 467 | C | ALA | 34 | 5.164 | 2.875 | -16.844 | 1.00 | 0.16 |
| ATOM | 468 | O | ALA | 34 | 4.954 | 1.677 | -16.847 | 1.00 | 0.17 |
| ATOM | 469 | N | PHE | 35 | 4.182 | 3.729 | -16.792 | 1.00 | 0.16 |
| ATOM | 470 | HN | PHE | 35 | 4.364 | 4.694 | -16.792 | 1.00 | 0.16 |
| ATOM | 471 | CA | PHE | 35 | 2.781 | 3.230 | -16.736 | 1.00 | 0.17 |
| ATOM | 472 | HA | PHE | 35 | 2.690 | 2.525 | -15.924 | 1.00 | 0.17 |
| ATOM | 473 | CB | PHE | 35 | 1.815 | 4.396 | -16.508 | 1.00 | 0.18 |
| ATOM | 474 | HB1 | PHE | 35 | 0.802 | 4.060 | -16.672 | 1.00 | 0.19 |
| ATOM | 475 | HB2 | PHE | 35 | 2.045 | 5.192 | -17.200 | 1.00 | 0.19 |
| ATOM | 476 | CG | PHE | 35 | 1.953 | 4.902 | -15.089 | 1.00 | 0.18 |
| ATOM | 477 | CD1 | PHE | 35 | 1.616 | 4.071 | -14.011 | 1.00 | 0.19 |
| ATOM | 478 | HD1 | PHE | 35 | 1.258 | 3.069 | -14.191 | 1.00 | 0.19 |
| ATOM | 479 | CD2 | PHE | 35 | 2.415 | 6.203 | -14.849 | 1.00 | 0.20 |
| ATOM | 480 | HD2 | PHE | 35 | 2.674 | 6.847 | -15.677 | 1.00 | 0.21 |
| ATOM | 481 | CE1 | PHE | 35 | 1.743 | 4.539 | -12.699 | 1.00 | 0.21 |
| ATOM | 482 | HE1 | PHE | 35 | 1.484 | 3.897 | -11.870 | 1.00 | 0.23 |
| ATOM | 483 | CE2 | PHE | 35 | 2.540 | 6.670 | -13.535 | 1.00 | 0.22 |
| ATOM | 484 | HE2 | PHE | 35 | 2.893 | 7.672 | -13.349 | 1.00 | 0.24 |
| ATOM | 485 | CZ | PHE | 35 | 2.205 | 5.838 | -12.460 | 1.00 | 0.22 |
| ATOM | 486 | HZ | PHE | 35 | 2.303 | 6.198 | -11.447 | 1.00 | 0.24 |
| ATOM | 487 | C | PHE | 35 | 2.432 | 2.524 | -18.048 | 1.00 | 0.18 |
| ATOM | 488 | O | PHE | 35 | 1.770 | 1.507 | -18.055 | 1.00 | 0.19 |
| ATOM | 489 | N | LYS | 36 | 2.864 | 3.053 | -19.162 | 1.00 | 0.19 |
| ATOM | 490 | HN | LYS | 36 | 3.394 | 3.878 | -19.144 | 1.00 | 0.19 |
| ATOM | 491 | CA | LYS | 36 | 2.535 | 2.399 | -20.460 | 1.00 | 0.22 |
| ATOM | 492 | HA | LYS | 36 | 1.462 | 2.358 | -20.574 | 1.00 | 0.23 |
| ATOM | 493 | CB | LYS | 36 | 3.135 | 3.205 | -21.614 | 1.00 | 0.24 |
| ATOM | 494 | HB1 | LYS | 36 | 3.045 | 2.641 | -22.530 | 1.00 | 0.27 |
| ATOM | 495 | HB2 | LYS | 36 | 4.178 | 3.400 | -21.412 | 1.00 | 0.24 |
| ATOM | 496 | CG | LYS | 36 | 2.384 | 4.530 | -21.758 | 1.00 | 0.27 |
| ATOM | 497 | HG1 | LYS | 36 | 2.471 | 5.097 | -20.844 | 1.00 | 0.69 |
| ATOM | 498 | HG2 | LYS | 36 | 1.341 | 4.332 | -21.963 | 1.00 | 0.68 |
| ATOM | 499 | CD | LYS | 36 | 2.988 | 5.332 | -22.913 | 1.00 | 0.75 |
| ATOM | 500 | HD1 | LYS | 36 | 2.898 | 4.766 | -23.828 | 1.00 | 1.39 |
| ATOM | 501 | HD2 | LYS | 36 | 4.032 | 5.525 | -22.710 | 1.00 | 1.34 |

11/75

| | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|---------|------|------|
| ATOM | 502 | CE | LYS | 36 | 2.243 | 6.659 | -23.065 | 1.00 | 1.15 |
| ATOM | 503 | HE1 | LYS | 36 | 2.728 | 7.415 | -22.464 | 1.00 | 1.64 |
| ATOM | 504 | HE2 | LYS | 36 | 1.221 | 6.540 | -22.736 | 1.00 | 1.61 |
| ATOM | 505 | NZ | LYS | 36 | 2.260 | 7.076 | -24.496 | 1.00 | 1.99 |
| ATOM | 506 | HZ1 | LYS | 36 | 2.628 | 6.298 | -25.079 | 1.00 | 2.51 |
| ATOM | 507 | HZ2 | LYS | 36 | 2.871 | 7.911 | -24.605 | 1.00 | 2.40 |
| ATOM | 508 | HZ3 | LYS | 36 | 1.295 | 7.309 | -24.801 | 1.00 | 2.38 |
| ATOM | 509 | C | LYS | 36 | 3.098 | 0.976 | -20.481 | 1.00 | 0.21 |
| ATOM | 510 | O | LYS | 36 | 2.446 | 0.053 | -20.927 | 1.00 | 0.23 |
| ATOM | 511 | N | LYS | 37 | 4.295 | 0.778 | -19.995 | 1.00 | 0.21 |
| ATOM | 512 | HN | LYS | 37 | 4.810 | 1.527 | -19.629 | 1.00 | 0.20 |
| ATOM | 513 | CA | LYS | 37 | 4.864 | -0.600 | -19.988 | 1.00 | 0.22 |
| ATOM | 514 | HA | LYS | 37 | 4.926 | -0.974 | -21.000 | 1.00 | 0.24 |
| ATOM | 515 | CB | LYS | 37 | 6.257 | -0.581 | -19.358 | 1.00 | 0.22 |
| ATOM | 516 | HB1 | LYS | 37 | 6.589 | -1.596 | -19.195 | 1.00 | 0.24 |
| ATOM | 517 | HB2 | LYS | 37 | 6.216 | -0.061 | -18.412 | 1.00 | 0.21 |
| ATOM | 518 | CG | LYS | 37 | 7.244 | 0.130 | -20.285 | 1.00 | 0.26 |
| ATOM | 519 | HG1 | LYS | 37 | 6.921 | 1.140 | -20.459 | 1.00 | 0.25 |
| ATOM | 520 | HG2 | LYS | 37 | 7.296 | -0.398 | -21.227 | 1.00 | 0.28 |
| ATOM | 521 | CD | LYS | 37 | 8.625 | 0.139 | -19.628 | 1.00 | 0.30 |
| ATOM | 522 | HD1 | LYS | 37 | 8.994 | -0.873 | -19.551 | 1.00 | 0.77 |
| ATOM | 523 | HD2 | LYS | 37 | 8.549 | 0.570 | -18.640 | 1.00 | 0.84 |
| ATOM | 524 | CE | LYS | 37 | 9.594 | 0.968 | -20.473 | 1.00 | 0.90 |
| ATOM | 525 | HE1 | LYS | 37 | 10.530 | 1.076 | -19.943 | 1.00 | 1.47 |
| ATOM | 526 | HE2 | LYS | 37 | 9.169 | 1.945 | -20.652 | 1.00 | 1.59 |
| ATOM | 527 | NZ | LYS | 37 | 9.836 | 0.286 | -21.774 | 1.00 | 1.77 |
| ATOM | 528 | HZ1 | LYS | 37 | 9.798 | 0.984 | -22.543 | 1.00 | 2.22 |
| ATOM | 529 | HZ2 | LYS | 37 | 9.106 | -0.439 | -21.926 | 1.00 | 2.28 |
| ATOM | 530 | HZ3 | LYS | 37 | 10.774 | -0.161 | -21.762 | 1.00 | 2.33 |
| ATOM | 531 | C | LYS | 37 | 3.955 | -1.506 | -19.158 | 1.00 | 0.20 |
| ATOM | 532 | O | LYS | 37 | 3.689 | -2.636 | -19.516 | 1.00 | 0.21 |
| ATOM | 533 | N | ALA | 38 | 3.479 | -1.013 | -18.046 | 1.00 | 0.19 |
| ATOM | 534 | HN | ALA | 38 | 3.711 | -0.098 | -17.777 | 1.00 | 0.19 |
| ATOM | 535 | CA | ALA | 38 | 2.589 | -1.838 | -17.182 | 1.00 | 0.18 |
| ATOM | 536 | HA | ALA | 38 | 3.116 | -2.727 | -16.870 | 1.00 | 0.19 |
| ATOM | 537 | CB | ALA | 38 | 2.183 | -1.030 | -15.949 | 1.00 | 0.19 |
| ATOM | 538 | HB1 | ALA | 38 | 2.831 | -0.172 | -15.851 | 1.00 | 1.05 |
| ATOM | 539 | HB2 | ALA | 38 | 2.270 | -1.649 | -15.068 | 1.00 | 1.00 |
| ATOM | 540 | HB3 | ALA | 38 | 1.161 | -0.698 | -16.057 | 1.00 | 1.06 |
| ATOM | 541 | C | ALA | 38 | 1.338 | -2.238 | -17.965 | 1.00 | 0.18 |
| ATOM | 542 | O | ALA | 38 | 0.967 | -3.392 | -18.012 | 1.00 | 0.19 |
| ATOM | 543 | N | PHE | 39 | 0.688 | -1.295 | -18.589 | 1.00 | 0.18 |
| ATOM | 544 | HN | PHE | 39 | 1.005 | -0.368 | -18.547 | 1.00 | 0.18 |
| ATOM | 545 | CA | PHE | 39 | -0.535 | -1.632 | -19.367 | 1.00 | 0.19 |
| ATOM | 546 | HA | PHE | 39 | -1.248 | -2.122 | -18.720 | 1.00 | 0.19 |
| ATOM | 547 | CB | PHE | 39 | -1.156 | -0.354 | -19.937 | 1.00 | 0.21 |
| ATOM | 548 | HB1 | PHE | 39 | -1.883 | -0.614 | -20.692 | 1.00 | 0.24 |
| ATOM | 549 | HB2 | PHE | 39 | -0.381 | 0.256 | -20.378 | 1.00 | 0.21 |
| ATOM | 550 | CG | PHE | 39 | -1.836 | 0.416 | -18.829 | 1.00 | 0.20 |
| ATOM | 551 | CD1 | PHE | 39 | -3.010 | -0.080 | -18.250 | 1.00 | 0.25 |
| ATOM | 552 | HD1 | PHE | 39 | -3.429 | -1.014 | -18.595 | 1.00 | 0.30 |
| ATOM | 553 | CD2 | PHE | 39 | -1.294 | 1.627 | -18.380 | 1.00 | 0.17 |
| ATOM | 554 | HD2 | PHE | 39 | -0.389 | 2.012 | -18.827 | 1.00 | 0.18 |
| ATOM | 555 | CE1 | PHE | 39 | -3.642 | 0.633 | -17.224 | 1.00 | 0.28 |
| ATOM | 556 | HE1 | PHE | 39 | -4.548 | 0.250 | -16.779 | 1.00 | 0.34 |
| ATOM | 557 | CE2 | PHE | 39 | -1.926 | 2.341 | -17.354 | 1.00 | 0.18 |
| ATOM | 558 | HE2 | PHE | 39 | -1.507 | 3.275 | -17.007 | 1.00 | 0.17 |
| ATOM | 559 | CZ | PHE | 39 | -3.099 | 1.843 | -16.776 | 1.00 | 0.23 |
| ATOM | 560 | HZ | PHE | 39 | -3.587 | 2.394 | -15.985 | 1.00 | 0.26 |
| ATOM | 561 | C | PHE | 39 | -0.154 | -2.571 | -20.508 | 1.00 | 0.18 |
| ATOM | 562 | O | PHE | 39 | -0.862 | -3.509 | -20.817 | 1.00 | 0.18 |
| ATOM | 563 | N | LYS | 40 | 0.963 | -2.330 | -21.136 | 1.00 | 0.19 |
| ATOM | 564 | HN | LYS | 40 | 1.522 | -1.570 | -20.870 | 1.00 | 0.19 |
| ATOM | 565 | CA | LYS | 40 | 1.388 | -3.214 | -22.254 | 1.00 | 0.19 |
| ATOM | 566 | HA | LYS | 40 | 0.642 | -3.186 | -23.031 | 1.00 | 0.20 |
| ATOM | 567 | CB | LYS | 40 | 2.730 | -2.707 | -22.804 | 1.00 | 0.21 |
| ATOM | 568 | HB1 | LYS | 40 | 3.466 | -2.723 | -22.014 | 1.00 | 0.21 |
| ATOM | 569 | HB2 | LYS | 40 | 2.610 | -1.692 | -23.155 | 1.00 | 0.25 |
| ATOM | 570 | CG | LYS | 40 | 3.218 | -3.588 | -23.966 | 1.00 | 0.25 |
| ATOM | 571 | HG1 | LYS | 40 | 3.337 | -4.604 | -23.621 | 1.00 | 0.46 |
| ATOM | 572 | HG2 | LYS | 40 | 4.171 | -3.218 | -24.314 | 1.00 | 0.46 |
| ATOM | 573 | CD | LYS | 40 | 2.213 | -3.560 | -25.121 | 1.00 | 0.38 |
| ATOM | 574 | HD1 | LYS | 40 | 1.840 | -2.555 | -25.253 | 1.00 | 0.54 |
| ATOM | 575 | HD2 | LYS | 40 | 1.392 | -4.227 | -24.905 | 1.00 | 0.56 |
| ATOM | 576 | CE | LYS | 40 | 2.903 | -4.019 | -26.407 | 1.00 | 0.40 |
| ATOM | 577 | HE1 | LYS | 40 | 3.776 | -4.604 | -26.158 | 1.00 | 1.07 |
| ATOM | 578 | HE2 | LYS | 40 | 3.168 | -3.167 | -26.005 | 1.00 | 1.07 |

12/75

| | | | | | | | | | |
|------|-----|------|-----|----|--------|---------|---------|------|------|
| ATOM | 579 | NZ | LYS | 40 | 1.958 | -4.852 | -27.203 | 1.00 | 1.40 |
| ATOM | 580 | HZ1 | LYS | 40 | 1.571 | -5.607 | -26.602 | 1.00 | 1.95 |
| ATOM | 581 | HZ2 | LYS | 40 | 2.464 | -5.274 | -28.009 | 1.00 | 1.92 |
| ATOM | 582 | HZ3 | LYS | 40 | 1.181 | -4.258 | -27.552 | 1.00 | 2.02 |
| ATOM | 583 | C | LYS | 40 | 1.553 | -4.648 | -21.740 | 1.00 | 0.17 |
| ATOM | 584 | O | LYS | 40 | 1.034 | -5.583 | -22.314 | 1.00 | 0.17 |
| ATOM | 585 | N | VAL | 41 | 2.271 | -4.828 | -20.663 | 1.00 | 0.17 |
| ATOM | 586 | HN | VAL | 41 | 2.681 | -4.060 | -20.214 | 1.00 | 0.18 |
| ATOM | 587 | CA | VAL | 41 | 2.468 | -6.204 | -20.116 | 1.00 | 0.16 |
| ATOM | 588 | HA | VAL | 41 | 2.953 | -6.816 | -20.862 | 1.00 | 0.17 |
| ATOM | 589 | CB | VAL | 41 | 3.350 | -6.143 | -18.868 | 1.00 | 0.18 |
| ATOM | 590 | HB | VAL | 41 | 2.966 | -5.393 | -18.192 | 1.00 | 0.41 |
| ATOM | 591 | CG1 | VAL | 41 | 3.343 | -7.508 | -18.175 | 1.00 | 0.44 |
| ATOM | 592 | HG11 | VAL | 41 | 2.420 | -7.631 | -17.629 | 1.00 | 1.16 |
| ATOM | 593 | HG12 | VAL | 41 | 4.176 | -7.571 | -17.490 | 1.00 | 1.18 |
| ATOM | 594 | HG13 | VAL | 41 | 3.429 | -8.289 | -18.916 | 1.00 | 1.11 |
| ATOM | 595 | CG2 | VAL | 41 | 4.781 | -5.785 | -19.277 | 1.00 | 0.43 |
| ATOM | 596 | HG21 | VAL | 41 | 5.132 | -6.492 | -20.013 | 1.00 | 1.12 |
| ATOM | 597 | HG22 | VAL | 41 | 5.423 | -5.820 | -18.411 | 1.00 | 1.11 |
| ATOM | 598 | HG23 | VAL | 41 | 4.797 | -4.790 | -19.697 | 1.00 | 1.19 |
| ATOM | 599 | C | VAL | 41 | 1.122 | -6.833 | -19.751 | 1.00 | 0.16 |
| ATOM | 600 | O | VAL | 41 | 0.887 | -7.999 | -19.996 | 1.00 | 0.17 |
| ATOM | 601 | N | TRP | 42 | 0.240 | -6.080 | -19.152 | 1.00 | 0.16 |
| ATOM | 602 | HN | TRP | 42 | 0.448 | -5.143 | -18.950 | 1.00 | 0.17 |
| ATOM | 603 | CA | TRP | 42 | -1.079 | -6.655 | -18.761 | 1.00 | 0.17 |
| ATOM | 604 | HA | TRP | 42 | -0.927 | -7.642 | -18.352 | 1.00 | 0.17 |
| ATOM | 605 | CB | TRP | 42 | -1.739 | -5.767 | -17.699 | 1.00 | 0.18 |
| ATOM | 606 | HB1 | TRP | 42 | -2.787 | -6.018 | -17.621 | 1.00 | 0.19 |
| ATOM | 607 | HB2 | TRP | 42 | -1.638 | -4.730 | -17.983 | 1.00 | 0.20 |
| ATOM | 608 | CG | TRP | 42 | -1.073 | -5.990 | -16.377 | 1.00 | 0.18 |
| ATOM | 609 | CD1 | TRP | 42 | -0.311 | -5.082 | -15.724 | 1.00 | 0.22 |
| ATOM | 610 | HD1 | TRP | 42 | -0.092 | -4.084 | -16.066 | 1.00 | 0.28 |
| ATOM | 611 | CD2 | TRP | 42 | -1.095 | -7.182 | -15.539 | 1.00 | 0.19 |
| ATOM | 612 | NE1 | TRP | 42 | 0.140 | -5.643 | -14.543 | 1.00 | 0.22 |
| ATOM | 613 | HE1 | TRP | 42 | 0.714 | -5.194 | -13.887 | 1.00 | 0.25 |
| ATOM | 614 | CE2 | TRP | 42 | -0.315 | -6.935 | -14.384 | 1.00 | 0.20 |
| ATOM | 615 | CE3 | TRP | 42 | -1.707 | -8.441 | -15.669 | 1.00 | 0.25 |
| ATOM | 616 | HE3 | TRP | 42 | -2.309 | -8.658 | -16.539 | 1.00 | 0.27 |
| ATOM | 617 | CZ2 | TRP | 42 | -0.149 | -7.903 | -13.393 | 1.00 | 0.24 |
| ATOM | 618 | HZ2 | TRP | 42 | 0.454 | -7.691 | -12.521 | 1.00 | 0.25 |
| ATOM | 619 | CZ3 | TRP | 42 | -1.543 | -9.418 | -14.673 | 1.00 | 0.31 |
| ATOM | 620 | HZ3 | TRP | 42 | -2.018 | -10.381 | -14.782 | 1.00 | 0.39 |
| ATOM | 621 | CH2 | TRP | 42 | -0.764 | -9.149 | -13.538 | 1.00 | 0.30 |
| ATOM | 622 | HH2 | TRP | 42 | -0.642 | -9.904 | -12.775 | 1.00 | 0.35 |
| ATOM | 623 | C | TRP | 42 | -1.991 | -6.754 | -19.985 | 1.00 | 0.17 |
| ATOM | 624 | O | TRP | 42 | -2.726 | -7.706 | -20.138 | 1.00 | 0.18 |
| ATOM | 625 | N | SER | 43 | -1.952 | -5.782 | -20.855 | 1.00 | 0.17 |
| ATOM | 626 | HN | SER | 43 | -1.352 | -5.021 | -20.713 | 1.00 | 0.17 |
| ATOM | 627 | CA | SER | 43 | -2.831 | -5.825 | -22.062 | 1.00 | 0.18 |
| ATOM | 628 | HA | SER | 43 | -3.846 | -6.028 | -21.759 | 1.00 | 0.19 |
| ATOM | 629 | CB | SER | 43 | -2.779 | -4.474 | -22.775 | 1.00 | 0.20 |
| ATOM | 630 | HB1 | SER | 43 | -2.965 | -3.683 | -22.059 | 1.00 | 0.21 |
| ATOM | 631 | HB2 | SER | 43 | -3.533 | -4.442 | -23.543 | 1.00 | 0.23 |
| ATOM | 632 | OG | SER | 43 | -1.499 | -4.304 | -23.368 | 1.00 | 0.21 |
| ATOM | 633 | HG | SER | 43 | -1.031 | -5.140 | -23.309 | 1.00 | 0.97 |
| ATOM | 634 | C | SER | 43 | -2.358 | -6.922 | -23.019 | 1.00 | 0.18 |
| ATOM | 635 | O | SER | 43 | -3.085 | -7.350 | -23.893 | 1.00 | 0.21 |
| ATOM | 636 | N | ASP | 44 | -1.148 | -7.379 | -22.866 | 1.00 | 0.17 |
| ATOM | 637 | HN | ASP | 44 | -0.575 | -7.019 | -22.156 | 1.00 | 0.18 |
| ATOM | 638 | CA | ASP | 44 | -0.632 | -8.445 | -23.770 | 1.00 | 0.18 |
| ATOM | 639 | HA | ASP | 44 | -0.650 | -8.086 | -24.788 | 1.00 | 0.19 |
| ATOM | 640 | CB | ASP | 44 | 0.809 | -8.793 | -23.386 | 1.00 | 0.20 |
| ATOM | 641 | HB1 | ASP | 44 | 1.117 | -9.683 | -23.915 | 1.00 | 0.21 |
| ATOM | 642 | HB2 | ASP | 44 | 0.864 | -8.969 | -22.322 | 1.00 | 0.22 |
| ATOM | 643 | CG | ASP | 44 | 1.734 | -7.635 | -23.760 | 1.00 | 0.24 |
| ATOM | 644 | OD1 | ASP | 44 | 1.340 | -6.833 | -24.591 | 1.00 | 0.85 |
| ATOM | 645 | OD2 | ASP | 44 | 2.820 | -7.568 | -23.209 | 1.00 | 0.84 |
| ATOM | 646 | C | ASP | 44 | -1.499 | -9.705 | -23.665 | 1.00 | 0.19 |
| ATOM | 647 | O | ASP | 44 | -1.753 | -10.366 | -24.653 | 1.00 | 0.21 |
| ATOM | 648 | N | VAL | 45 | -1.927 | -10.058 | -22.475 | 1.00 | 0.21 |
| ATOM | 649 | HN | VAL | 45 | -1.689 | -9.519 | -21.693 | 1.00 | 0.21 |
| ATOM | 650 | CA | VAL | 45 | -2.749 | -11.299 | -22.302 | 1.00 | 0.26 |
| ATOM | 651 | HA | VAL | 45 | -2.833 | -11.811 | -23.247 | 1.00 | 0.28 |
| ATOM | 652 | CB | VAL | 45 | -2.045 | -12.222 | -21.303 | 1.00 | 0.30 |
| ATOM | 653 | HB | VAL | 45 | -2.645 | -13.107 | -21.146 | 1.00 | 0.37 |
| ATOM | 654 | CG1 | VAL | 45 | -0.678 | -12.626 | -21.866 | 1.00 | 0.36 |
| ATOM | 655 | HG11 | VAL | 45 | -0.210 | -11.766 | -22.322 | 1.00 | 0.22 |

13/75

| | | | | | | | | | |
|------|-----|------|-----|----|---------|---------|---------|------|------|
| ATOM | 656 | HG12 | VAL | 45 | -0.810 | -13.400 | -22.607 | 1.00 | 1.02 |
| ATOM | 657 | HG13 | VAL | 45 | -0.051 | -12.995 | -21.068 | 1.00 | 1.13 |
| ATOM | 658 | CG2 | VAL | 45 | -1.855 | -11.486 | -19.973 | 1.00 | 0.32 |
| ATOM | 659 | HG21 | VAL | 45 | -2.819 | -11.303 | -19.524 | 1.00 | 0.96 |
| ATOM | 660 | HG22 | VAL | 45 | -1.356 | -10.545 | -20.149 | 1.00 | 1.09 |
| ATOM | 661 | HG23 | VAL | 45 | -1.258 | -12.091 | -19.305 | 1.00 | 1.11 |
| ATOM | 662 | C | VAL | 45 | -4.160 | -10.966 | -21.790 | 1.00 | 0.29 |
| ATOM | 663 | O | VAL | 45 | -4.837 | -11.819 | -21.249 | 1.00 | 0.64 |
| ATOM | 664 | N | THR | 46 | -4.619 | -9.748 | -21.963 | 1.00 | 0.36 |
| ATOM | 665 | HN | THR | 46 | -4.062 | -9.076 | -22.409 | 1.00 | 0.65 |
| ATOM | 666 | CA | THR | 46 | -5.998 | -9.382 | -21.491 | 1.00 | 0.38 |
| ATOM | 667 | HA | THR | 46 | -6.567 | -10.277 | -21.320 | 1.00 | 0.44 |
| ATOM | 668 | CB | THR | 46 | -5.912 | -8.577 | -20.186 | 1.00 | 0.39 |
| ATOM | 669 | HB | THR | 46 | -6.889 | -8.193 | -19.943 | 1.00 | 0.46 |
| ATOM | 670 | OG1 | THR | 46 | -5.018 | -7.491 | -20.358 | 1.00 | 0.36 |
| ATOM | 671 | HG1 | THR | 46 | -5.532 | -6.719 | -20.608 | 1.00 | 0.94 |
| ATOM | 672 | CG2 | THR | 46 | -5.430 | -9.461 | -19.036 | 1.00 | 0.43 |
| ATOM | 673 | HG21 | THR | 46 | -4.929 | -10.327 | -19.429 | 1.00 | 1.08 |
| ATOM | 674 | HG22 | THR | 46 | -6.277 | -9.775 | -18.445 | 1.00 | 1.15 |
| ATOM | 675 | HG23 | THR | 46 | -4.746 | -8.901 | -18.415 | 1.00 | 1.05 |
| ATOM | 676 | C | THR | 46 | -6.668 | -8.482 | -22.553 | 1.00 | 0.32 |
| ATOM | 677 | O | THR | 46 | -6.124 | -7.450 | -22.892 | 1.00 | 0.32 |
| ATOM | 678 | N | PRO | 47 | -7.833 | -8.829 | -23.084 | 1.00 | 0.30 |
| ATOM | 679 | CA | PRO | 47 | -8.479 | -7.951 | -24.100 | 1.00 | 0.30 |
| ATOM | 680 | HA | PRO | 47 | -7.820 | -7.790 | -24.936 | 1.00 | 0.33 |
| ATOM | 681 | CB | PRO | 47 | -9.687 | -8.773 | -24.546 | 1.00 | 0.35 |
| ATOM | 682 | HB1 | PRO | 47 | -9.541 | -9.110 | -25.561 | 1.00 | 0.40 |
| ATOM | 683 | HB2 | PRO | 47 | -10.579 | -8.166 | -24.489 | 1.00 | 0.37 |
| ATOM | 684 | CG | PRO | 47 | -9.825 | -9.986 | -23.621 | 1.00 | 0.35 |
| ATOM | 685 | HG1 | PRO | 47 | -9.916 | -10.885 | -24.212 | 1.00 | 0.42 |
| ATOM | 686 | HG2 | PRO | 47 | -10.703 | -9.869 | -23.001 | 1.00 | 0.34 |
| ATOM | 687 | CD | PRO | 47 | -8.576 | -10.077 | -22.739 | 1.00 | 0.33 |
| ATOM | 688 | HD2 | PRO | 47 | -8.853 | -10.091 | -21.692 | 1.00 | 0.31 |
| ATOM | 689 | HD1 | PRO | 47 | -7.993 | -10.946 | -22.999 | 1.00 | 0.39 |
| ATOM | 690 | C | PRO | 47 | -8.933 | -6.614 | -23.506 | 1.00 | 0.25 |
| ATOM | 691 | O | PRO | 47 | -9.744 | -5.914 | -24.080 | 1.00 | 0.26 |
| ATOM | 692 | N | LEU | 48 | -8.418 | -6.252 | -22.362 | 1.00 | 0.26 |
| ATOM | 693 | HN | LEU | 48 | -7.766 | -6.828 | -21.912 | 1.00 | 0.29 |
| ATOM | 694 | CA | LEU | 48 | -8.827 | -4.960 | -21.742 | 1.00 | 0.26 |
| ATOM | 695 | HA | LEU | 48 | -9.904 | -4.905 | -21.696 | 1.00 | 0.27 |
| ATOM | 696 | CB | LEU | 48 | -8.241 | -4.858 | -20.329 | 1.00 | 0.31 |
| ATOM | 697 | HB1 | LEU | 48 | -8.476 | -3.892 | -19.909 | 1.00 | 0.34 |
| ATOM | 698 | HB2 | LEU | 48 | -7.167 | -4.968 | -20.385 | 1.00 | 0.33 |
| ATOM | 699 | CG | LEU | 48 | -8.816 | -5.964 | -19.434 | 1.00 | 0.34 |
| ATOM | 700 | HG | LEU | 48 | -8.808 | -6.900 | -19.972 | 1.00 | 0.32 |
| ATOM | 701 | CD1 | LEU | 48 | -7.952 | -6.091 | -18.177 | 1.00 | 0.41 |
| ATOM | 702 | HD11 | LEU | 48 | -8.002 | -5.171 | -17.613 | 1.00 | 1.11 |
| ATOM | 703 | HD12 | LEU | 48 | -6.928 | -6.283 | -18.462 | 1.00 | 1.05 |
| ATOM | 704 | HD13 | LEU | 48 | -8.315 | -6.906 | -17.570 | 1.00 | 1.15 |
| ATOM | 705 | CD2 | LEU | 48 | -10.255 | -5.628 | -19.016 | 1.00 | 0.36 |
| ATOM | 706 | HD21 | LEU | 48 | -10.569 | -4.707 | -19.478 | 1.00 | 1.10 |
| ATOM | 707 | HD22 | LEU | 48 | -10.299 | -5.524 | -17.942 | 1.00 | 1.09 |
| ATOM | 708 | HD23 | LEU | 48 | -10.912 | -6.428 | -19.325 | 1.00 | 1.04 |
| ATOM | 709 | C | LEU | 48 | -8.289 | -3.806 | -22.589 | 1.00 | 0.25 |
| ATOM | 710 | O | LEU | 48 | -7.174 | -3.849 | -23.071 | 1.00 | 0.26 |
| ATOM | 711 | N | ASN | 49 | -9.073 | -2.775 | -22.762 | 1.00 | 0.25 |
| ATOM | 712 | HN | ASN | 49 | -9.964 | -2.770 | -22.355 | 1.00 | 0.26 |
| ATOM | 713 | CA | ASN | 49 | -8.622 | -1.604 | -23.568 | 1.00 | 0.25 |
| ATOM | 714 | HA | ASN | 49 | -7.703 | -1.842 | -24.082 | 1.00 | 0.27 |
| ATOM | 715 | CB | ASN | 49 | -9.700 | -1.245 | -24.593 | 1.00 | 0.28 |
| ATOM | 716 | HB1 | ASN | 49 | -9.390 | -0.375 | -25.153 | 1.00 | 0.30 |
| ATOM | 717 | HB2 | ASN | 49 | -10.628 | -1.033 | -24.081 | 1.00 | 0.28 |
| ATOM | 718 | CG | ASN | 49 | -9.902 | -2.419 | -25.553 | 1.00 | 0.32 |
| ATOM | 719 | OD1 | ASN | 49 | -9.798 | -3.564 | -25.161 | 1.00 | 1.10 |
| ATOM | 720 | ND2 | ASN | 49 | -10.186 | -2.182 | -26.804 | 1.00 | 1.14 |
| ATOM | 721 | HD21 | ASN | 49 | -10.268 | -1.258 | -27.121 | 1.00 | 1.94 |
| ATOM | 722 | HD22 | ASN | 49 | -10.317 | -2.927 | -27.427 | 1.00 | 1.14 |
| ATOM | 723 | C | ASN | 49 | -8.391 | -0.417 | -22.633 | 1.00 | 0.24 |
| ATOM | 724 | O | ASN | 49 | -9.290 | 0.016 | -21.939 | 1.00 | 0.23 |
| ATOM | 725 | N | PHE | 50 | -7.192 | 0.107 | -22.606 | 1.00 | 0.24 |
| ATOM | 726 | HN | PHE | 50 | -6.485 | -0.264 | -23.173 | 1.00 | 0.26 |
| ATOM | 727 | CA | PHE | 50 | -6.896 | 1.263 | -21.710 | 1.00 | 0.23 |
| ATOM | 728 | HA | PHE | 50 | -7.688 | 1.380 | -20.985 | 1.00 | 0.21 |
| ATOM | 729 | CB | PHE | 50 | -5.574 | 1.016 | -20.981 | 1.00 | 0.24 |
| ATOM | 730 | HB1 | PHE | 50 | -5.357 | 1.853 | -20.334 | 1.00 | 0.25 |
| ATOM | 731 | HB2 | PHE | 50 | -4.780 | 0.907 | -21.705 | 1.00 | 0.27 |
| ATOM | 732 | CG | PHE | 50 | -5.676 | -0.243 | -20.154 | 1.00 | 0.23 |

14/75

| | | | | | | | | | |
|------|-----|------|-----|----|---------|--------|---------|------|------|
| ATOM | 733 | CD1 | PHE | 50 | -6.266 | -0.201 | -18.886 | 1.00 | 0.25 |
| ATOM | 734 | HD1 | PHE | 50 | -6.652 | 0.731 | -18.500 | 1.00 | 0.28 |
| ATOM | 735 | CD2 | PHE | 50 | -5.176 | -1.451 | -20.654 | 1.00 | 0.22 |
| ATOM | 736 | HD2 | PHE | 50 | -4.720 | -1.483 | -21.633 | 1.00 | 0.23 |
| ATOM | 737 | CE1 | PHE | 50 | -6.358 | -1.368 | -18.117 | 1.00 | 0.25 |
| ATOM | 738 | HE1 | PHE | 50 | -6.813 | -1.336 | -17.139 | 1.00 | 0.28 |
| ATOM | 739 | CE2 | PHE | 50 | -5.267 | -2.618 | -19.886 | 1.00 | 0.23 |
| ATOM | 740 | HE2 | PHE | 50 | -4.881 | -3.550 | -20.272 | 1.00 | 0.25 |
| ATOM | 741 | CZ | PHE | 50 | -5.858 | -2.576 | -18.618 | 1.00 | 0.24 |
| ATOM | 742 | HZ | PHE | 50 | -5.928 | -3.476 | -18.025 | 1.00 | 0.25 |
| ATOM | 743 | C | PHE | 50 | -6.777 | 2.538 | -22.545 | 1.00 | 0.26 |
| ATOM | 744 | O | PHE | 50 | -6.028 | 2.596 | -23.501 | 1.00 | 0.31 |
| ATOM | 745 | N | THR | 51 | -7.517 | 3.555 | -22.184 | 1.00 | 0.24 |
| ATOM | 746 | HN | THR | 51 | -8.109 | 3.468 | -21.413 | 1.00 | 0.22 |
| ATOM | 747 | CA | THR | 51 | -7.470 | 4.842 | -22.940 | 1.00 | 0.27 |
| ATOM | 748 | HA | THR | 51 | -6.775 | 4.762 | -23.762 | 1.00 | 0.31 |
| ATOM | 749 | CB | THR | 51 | -8.868 | 5.153 | -23.483 | 1.00 | 0.30 |
| ATOM | 750 | HB | THR | 51 | -9.562 | 5.248 | -22.663 | 1.00 | 0.29 |
| ATOM | 751 | OG1 | THR | 51 | -9.283 | 4.100 | -24.341 | 1.00 | 0.35 |
| ATOM | 752 | HG1 | THR | 51 | -9.638 | 4.491 | -25.142 | 1.00 | 0.84 |
| ATOM | 753 | CG2 | THR | 51 | -8.835 | 6.464 | -24.273 | 1.00 | 0.34 |
| ATOM | 754 | HG21 | THR | 51 | -9.805 | 6.640 | -24.716 | 1.00 | 1.02 |
| ATOM | 755 | HG22 | THR | 51 | -8.092 | 6.394 | -25.053 | 1.00 | 1.07 |
| ATOM | 756 | HG23 | THR | 51 | -8.588 | 7.280 | -23.611 | 1.00 | 1.13 |
| ATOM | 757 | C | THR | 51 | -7.024 | 5.969 | -22.001 | 1.00 | 0.25 |
| ATOM | 758 | O | THR | 51 | -7.553 | 6.139 | -20.920 | 1.00 | 0.22 |
| ATOM | 759 | N | ARG | 52 | -6.054 | 6.740 | -22.411 | 1.00 | 0.29 |
| ATOM | 760 | HN | ARG | 52 | -5.645 | 6.583 | -23.287 | 1.00 | 0.32 |
| ATOM | 761 | CA | ARG | 52 | -5.566 | 7.861 | -21.556 | 1.00 | 0.29 |
| ATOM | 762 | HA | ARG | 52 | -5.591 | 7.563 | -20.518 | 1.00 | 0.27 |
| ATOM | 763 | CB | ARG | 52 | -4.128 | 8.201 | -21.955 | 1.00 | 0.35 |
| ATOM | 764 | HB1 | ARG | 52 | -4.125 | 8.654 | -22.935 | 1.00 | 0.39 |
| ATOM | 765 | HB2 | ARG | 52 | -3.539 | 7.295 | -21.977 | 1.00 | 0.38 |
| ATOM | 766 | CG | ARG | 52 | -3.521 | 9.177 | -20.945 | 1.00 | 0.39 |
| ATOM | 767 | HG1 | ARG | 52 | -3.645 | 8.787 | -19.946 | 1.00 | 0.71 |
| ATOM | 768 | HG2 | ARG | 52 | -4.017 | 10.134 | -21.025 | 1.00 | 0.57 |
| ATOM | 769 | CD | ARG | 52 | -2.030 | 9.345 | -21.244 | 1.00 | 0.79 |
| ATOM | 770 | HD1 | ARG | 52 | -1.825 | 9.001 | -22.248 | 1.00 | 1.45 |
| ATOM | 771 | HD2 | ARG | 52 | -1.453 | 8.763 | -20.543 | 1.00 | 1.39 |
| ATOM | 772 | NE | ARG | 52 | -1.656 | 10.782 | -21.120 | 1.00 | 1.47 |
| ATOM | 773 | HE | ARG | 52 | -2.354 | 11.468 | -21.073 | 1.00 | 2.06 |
| ATOM | 774 | CZ | ARG | 52 | -0.398 | 11.127 | -21.071 | 1.00 | 2.09 |
| ATOM | 775 | NH1 | ARG | 52 | -0.070 | 12.385 | -20.960 | 1.00 | 3.05 |
| ATOM | 776 | HH11 | ARG | 52 | -0.782 | 13.084 | -20.911 | 1.00 | 3.45 |
| ATOM | 777 | HH12 | ARG | 52 | 0.894 | 12.649 | -20.923 | 1.00 | 3.60 |
| ATOM | 778 | NH2 | ARG | 52 | 0.532 | 10.213 | -21.138 | 1.00 | 2.31 |
| ATOM | 779 | HH21 | ARG | 52 | 0.281 | 9.249 | -21.226 | 1.00 | 2.16 |
| ATOM | 780 | HH22 | ARG | 52 | 1.496 | 10.477 | -21.102 | 1.00 | 3.05 |
| ATOM | 781 | C | ARG | 52 | -6.460 | 9.090 | -21.758 | 1.00 | 0.29 |
| ATOM | 782 | O | ARG | 52 | -6.719 | 9.495 | -22.875 | 1.00 | 0.33 |
| ATOM | 783 | N | LEU | 53 | -6.928 | 9.689 | -20.689 | 1.00 | 0.26 |
| ATOM | 784 | HN | LEU | 53 | -6.702 | 9.345 | -19.798 | 1.00 | 0.25 |
| ATOM | 785 | CA | LEU | 53 | -7.803 | 10.896 | -20.822 | 1.00 | 0.29 |
| ATOM | 786 | HA | LEU | 53 | -8.167 | 10.972 | -21.835 | 1.00 | 0.32 |
| ATOM | 787 | CB | LEU | 53 | -8.992 | 10.784 | -19.862 | 1.00 | 0.28 |
| ATOM | 788 | HB1 | LEU | 53 | -9.579 | 11.688 | -19.908 | 1.00 | 0.31 |
| ATOM | 789 | HB2 | LEU | 53 | -8.624 | 10.648 | -18.855 | 1.00 | 0.28 |
| ATOM | 790 | CG | LEU | 53 | -9.866 | 9.587 | -20.249 | 1.00 | 0.28 |
| ATOM | 791 | HG | LEU | 53 | -9.264 | 8.690 | -20.246 | 1.00 | 0.29 |
| ATOM | 792 | CD1 | LEU | 53 | -10.999 | 9.440 | -19.232 | 1.00 | 0.29 |
| ATOM | 793 | HD11 | LEU | 53 | -11.606 | 8.585 | -19.487 | 1.00 | 0.95 |
| ATOM | 794 | HD12 | LEU | 53 | -11.610 | 10.331 | -19.243 | 1.00 | 1.05 |
| ATOM | 795 | HD13 | LEU | 53 | -10.581 | 9.303 | -18.247 | 1.00 | 1.07 |
| ATOM | 796 | CD2 | LEU | 53 | -10.463 | 9.799 | -21.646 | 1.00 | 0.36 |
| ATOM | 797 | HD21 | LEU | 53 | -10.523 | 10.856 | -21.860 | 1.00 | 1.01 |
| ATOM | 798 | HD22 | LEU | 53 | -11.453 | 9.370 | -21.685 | 1.00 | 1.09 |
| ATOM | 799 | HD23 | LEU | 53 | -9.835 | 9.319 | -22.382 | 1.00 | 1.14 |
| ATOM | 800 | C | LEU | 53 | -7.000 | 12.154 | -20.483 | 1.00 | 0.33 |
| ATOM | 801 | O | LEU | 53 | -6.315 | 12.218 | -19.482 | 1.00 | 0.34 |
| ATOM | 802 | N | HIS | 54 | -7.080 | 13.154 | -21.319 | 1.00 | 0.41 |
| ATOM | 803 | HN | HIS | 54 | -7.637 | 13.075 | -22.121 | 1.00 | 0.45 |
| ATOM | 804 | CA | HIS | 54 | -6.324 | 14.413 | -21.062 | 1.00 | 0.47 |
| ATOM | 805 | HA | HIS | 54 | -5.292 | 14.183 | -20.851 | 1.00 | 0.54 |
| ATOM | 806 | CB | HIS | 54 | -6.407 | 15.314 | -22.297 | 1.00 | 0.60 |
| ATOM | 807 | HB1 | HIS | 54 | -6.018 | 16.291 | -22.052 | 1.00 | 0.64 |
| ATOM | 808 | HB2 | HIS | 54 | -7.438 | 15.407 | -22.603 | 1.00 | 0.61 |
| ATOM | 809 | CG | HIS | 54 | -5.602 | 14.726 | -23.426 | 1.00 | 0.74 |

15/75

| | | | | | | | | | |
|------|-----|------|-----|----|---------|--------|---------|------|------|
| ATOM | 810 | ND1 | HIS | 54 | -5.645 | 15.254 | -24.707 | 1.00 | 1.35 |
| ATOM | 811 | HD1 | HIS | 54 | -6.172 | 16.028 | -24.996 | 1.00 | 1.86 |
| ATOM | 812 | CD2 | HIS | 54 | -4.740 | 13.656 | -23.493 | 1.00 | 0.86 |
| ATOM | 813 | HD2 | HIS | 54 | -4.480 | 13.010 | -22.668 | 1.00 | 1.34 |
| ATOM | 814 | CE1 | HIS | 54 | -4.834 | 14.512 | -25.481 | 1.00 | 1.33 |
| ATOM | 815 | HE1 | HIS | 54 | -4.670 | 14.692 | -26.533 | 1.00 | 1.83 |
| ATOM | 816 | NE2 | HIS | 54 | -4.257 | 13.525 | -24.792 | 1.00 | 0.92 |
| ATOM | 817 | C | HIS | 54 | -6.933 | 15.154 | -19.867 | 1.00 | 0.43 |
| ATOM | 818 | O | HIS | 54 | -6.230 | 15.714 | -19.051 | 1.00 | 0.49 |
| ATOM | 819 | N | ASP | 55 | -8.236 | 15.172 | -19.767 | 1.00 | 0.42 |
| ATOM | 820 | HN | ASP | 55 | -8.784 | 14.719 | -20.442 | 1.00 | 0.45 |
| ATOM | 821 | CA | ASP | 55 | -8.892 | 15.892 | -18.635 | 1.00 | 0.49 |
| ATOM | 822 | HA | ASP | 55 | -8.217 | 15.938 | -17.796 | 1.00 | 0.54 |
| ATOM | 823 | CB | ASP | 55 | -9.251 | 17.314 | -19.073 | 1.00 | 0.65 |
| ATOM | 824 | HB1 | ASP | 55 | -9.876 | 17.774 | -18.323 | 1.00 | 0.75 |
| ATOM | 825 | HB2 | ASP | 55 | -9.783 | 17.277 | -20.013 | 1.00 | 0.68 |
| ATOM | 826 | CG | ASP | 55 | -7.974 | 18.140 | -19.244 | 1.00 | 0.71 |
| ATOM | 827 | OD1 | ASP | 55 | -7.978 | 19.037 | -20.071 | 1.00 | 1.19 |
| ATOM | 828 | OD2 | ASP | 55 | -7.018 | 17.870 | -18.536 | 1.00 | 1.28 |
| ATOM | 829 | C | ASP | 55 | -10.167 | 15.156 | -18.223 | 1.00 | 0.45 |
| ATOM | 830 | O | ASP | 55 | -10.638 | 14.273 | -18.912 | 1.00 | 0.44 |
| ATOM | 831 | N | GLY | 56 | -10.728 | 15.518 | -17.100 | 1.00 | 0.46 |
| ATOM | 832 | HN | GLY | 56 | -10.328 | 16.233 | -16.563 | 1.00 | 0.50 |
| ATOM | 833 | CA | GLY | 56 | -11.975 | 14.848 | -16.632 | 1.00 | 0.44 |
| ATOM | 834 | HA1 | GLY | 56 | -12.482 | 14.399 | -17.472 | 1.00 | 0.44 |
| ATOM | 835 | HA2 | GLY | 56 | -12.622 | 15.579 | -16.169 | 1.00 | 0.48 |
| ATOM | 836 | C | GLY | 56 | -11.624 | 13.760 | -15.614 | 1.00 | 0.40 |
| ATOM | 837 | O | GLY | 56 | -10.473 | 13.543 | -15.294 | 1.00 | 0.42 |
| ATOM | 838 | N | ILE | 57 | -12.613 | 13.078 | -15.105 | 1.00 | 0.37 |
| ATOM | 839 | HN | ILE | 57 | -13.533 | 13.275 | -15.380 | 1.00 | 0.39 |
| ATOM | 840 | CA | ILE | 57 | -12.352 | 12.002 | -14.106 | 1.00 | 0.35 |
| ATOM | 841 | HA | ILE | 57 | -11.406 | 12.184 | -13.616 | 1.00 | 0.38 |
| ATOM | 842 | CB | ILE | 57 | -13.473 | 12.000 | -13.064 | 1.00 | 0.41 |
| ATOM | 843 | HB | ILE | 57 | -14.415 | 11.820 | -13.561 | 1.00 | 0.42 |
| ATOM | 844 | CG1 | ILE | 57 | -13.508 | 13.363 | -12.360 | 1.00 | 0.48 |
| ATOM | 845 | HG11 | ILE | 57 | -13.512 | 14.148 | -13.101 | 1.00 | 0.48 |
| ATOM | 846 | HG12 | ILE | 57 | -12.631 | 13.465 | -11.737 | 1.00 | 0.51 |
| ATOM | 847 | CG2 | ILE | 57 | -13.216 | 10.896 | -12.037 | 1.00 | 0.44 |
| ATOM | 848 | HG21 | ILE | 57 | -13.315 | 9.932 | -12.513 | 1.00 | 1.19 |
| ATOM | 849 | HG22 | ILE | 57 | -13.934 | 10.977 | -11.235 | 1.00 | 1.09 |
| ATOM | 850 | HG23 | ILE | 57 | -12.218 | 11.000 | -11.639 | 1.00 | 1.04 |
| ATOM | 851 | CD1 | ILE | 57 | -14.765 | 13.484 | -11.488 | 1.00 | 0.56 |
| ATOM | 852 | HD11 | ILE | 57 | -15.459 | 12.693 | -11.728 | 1.00 | 1.08 |
| ATOM | 853 | HD12 | ILE | 57 | -15.235 | 14.439 | -11.668 | 1.00 | 1.24 |
| ATOM | 854 | HD13 | ILE | 57 | -14.487 | 13.413 | -10.447 | 1.00 | 1.14 |
| ATOM | 855 | C | ILE | 57 | -12.307 | 10.647 | -14.817 | 1.00 | 0.30 |
| ATOM | 856 | O | ILE | 57 | -13.139 | 10.353 | -15.653 | 1.00 | 0.31 |
| ATOM | 857 | N | ALA | 58 | -11.337 | 9.828 | -14.493 | 1.00 | 0.26 |
| ATOM | 858 | HN | ALA | 58 | -10.679 | 10.096 | -13.817 | 1.00 | 0.27 |
| ATOM | 859 | CA | ALA | 58 | -11.221 | 8.489 | -15.148 | 1.00 | 0.23 |
| ATOM | 860 | HA | ALA | 58 | -11.957 | 8.398 | -15.932 | 1.00 | 0.25 |
| ATOM | 861 | CB | ALA | 58 | -9.824 | 8.339 | -15.749 | 1.00 | 0.23 |
| ATOM | 862 | HB1 | ALA | 58 | -9.843 | 7.585 | -16.522 | 1.00 | 0.97 |
| ATOM | 863 | HB2 | ALA | 58 | -9.129 | 8.044 | -14.976 | 1.00 | 1.11 |
| ATOM | 864 | HB3 | ALA | 58 | -9.513 | 9.280 | -16.172 | 1.00 | 1.03 |
| ATOM | 865 | C | ALA | 58 | -11.443 | 7.387 | -14.114 | 1.00 | 0.23 |
| ATOM | 866 | O | ALA | 58 | -11.389 | 7.617 | -12.922 | 1.00 | 0.27 |
| ATOM | 867 | N | ASP | 59 | -11.701 | 6.189 | -14.564 | 1.00 | 0.25 |
| ATOM | 868 | HN | ASP | 59 | -11.744 | 6.028 | -15.530 | 1.00 | 0.28 |
| ATOM | 869 | CA | ASP | 59 | -11.934 | 5.069 | -13.613 | 1.00 | 0.27 |
| ATOM | 870 | HA | ASP | 59 | -12.788 | 5.296 | -12.991 | 1.00 | 0.34 |
| ATOM | 871 | CB | ASP | 59 | -12.207 | 3.785 | -14.400 | 1.00 | 0.33 |
| ATOM | 872 | HB1 | ASP | 59 | -12.203 | 2.942 | -13.725 | 1.00 | 0.34 |
| ATOM | 873 | HB2 | ASP | 59 | -11.438 | 3.651 | -15.147 | 1.00 | 0.32 |
| ATOM | 874 | CG | ASP | 59 | -13.572 | 3.880 | -15.084 | 1.00 | 0.44 |
| ATOM | 875 | OD1 | ASP | 59 | -13.791 | 3.139 | -16.028 | 1.00 | 1.20 |
| ATOM | 876 | OD2 | ASP | 59 | -14.374 | 4.691 | -14.653 | 1.00 | 1.14 |
| ATOM | 877 | C | ASP | 59 | -10.700 | 4.863 | -12.731 | 1.00 | 0.22 |
| ATOM | 878 | O | ASP | 59 | -10.806 | 4.767 | -11.524 | 1.00 | 0.27 |
| ATOM | 879 | N | ILE | 60 | -9.534 | 4.780 | -13.326 | 1.00 | 0.18 |
| ATOM | 880 | HN | ILE | 60 | -9.478 | 4.850 | -14.302 | 1.00 | 0.20 |
| ATOM | 881 | CA | ILE | 60 | -8.291 | 4.561 | -12.523 | 1.00 | 0.22 |
| ATOM | 882 | HA | ILE | 60 | -8.554 | 4.303 | -11.512 | 1.00 | 0.28 |
| ATOM | 883 | CB | ILE | 60 | -7.502 | 3.404 | -13.155 | 1.00 | 0.27 |
| ATOM | 884 | HB | ILE | 60 | -7.255 | 3.655 | -14.175 | 1.00 | 0.28 |
| ATOM | 885 | CG1 | ILE | 60 | -8.377 | 2.146 | -13.136 | 1.00 | 0.30 |

16/75

| | | | | | | | | | |
|------|-----|------|-----|----|--------|--------|---------|------|------|
| ATOM | 887 | HG12 | ILE | 60 | -8.541 | 1.839 | -12.113 | 1.00 | 0.36 |
| ATOM | 888 | CG2 | ILE | 60 | -6.210 | 3.127 | -12.369 | 1.00 | 0.39 |
| ATOM | 889 | HG21 | ILE | 60 | -6.456 | 2.704 | -11.409 | 1.00 | 1.05 |
| ATOM | 890 | HG22 | ILE | 60 | -5.658 | 4.043 | -12.228 | 1.00 | 1.10 |
| ATOM | 891 | HG23 | ILE | 60 | -5.600 | 2.428 | -12.921 | 1.00 | 1.12 |
| ATOM | 892 | CD1 | ILE | 60 | -7.688 | 1.015 | -13.904 | 1.00 | 0.38 |
| ATOM | 893 | HD11 | ILE | 60 | -7.209 | 1.413 | -14.786 | 1.00 | 1.07 |
| ATOM | 894 | HD12 | ILE | 60 | -8.424 | 0.280 | -14.196 | 1.00 | 1.14 |
| ATOM | 895 | HD13 | ILE | 60 | -6.948 | 0.549 | -13.270 | 1.00 | 1.04 |
| ATOM | 896 | C | ILE | 60 | -7.438 | 5.834 | -12.518 | 1.00 | 0.20 |
| ATOM | 897 | O | ILE | 60 | -6.731 | 6.115 | -13.464 | 1.00 | 0.25 |
| ATOM | 898 | N | MET | 61 | -7.473 | 6.585 | -11.448 | 1.00 | 0.20 |
| ATOM | 899 | HN | MET | 61 | -8.033 | 6.326 | -10.687 | 1.00 | 0.25 |
| ATOM | 900 | CA | MET | 61 | -6.641 | 7.822 | -11.373 | 1.00 | 0.20 |
| ATOM | 901 | HA | MET | 61 | -6.327 | 8.102 | -12.366 | 1.00 | 0.19 |
| ATOM | 902 | CB | MET | 61 | -7.464 | 8.963 | -10.773 | 1.00 | 0.24 |
| ATOM | 903 | HB1 | MET | 61 | -8.331 | 9.137 | -11.392 | 1.00 | 0.35 |
| ATOM | 904 | HB2 | MET | 61 | -6.860 | 9.856 | -10.743 | 1.00 | 0.33 |
| ATOM | 905 | CG | MET | 61 | -7.918 | 8.604 | -9.358 | 1.00 | 0.31 |
| ATOM | 906 | HG1 | MET | 61 | -7.146 | 8.870 | -8.653 | 1.00 | 0.66 |
| ATOM | 907 | HG2 | MET | 61 | -8.112 | 7.544 | -9.300 | 1.00 | 0.67 |
| ATOM | 908 | SD | MET | 61 | -9.433 | 9.519 | -8.967 | 1.00 | 0.54 |
| ATOM | 909 | CE | MET | 61 | -8.878 | 11.154 | -9.516 | 1.00 | 0.40 |
| ATOM | 910 | HE1 | MET | 61 | -9.492 | 11.914 | -9.056 | 1.00 | 1.06 |
| ATOM | 911 | HE2 | MET | 61 | -8.968 | 11.227 | -10.589 | 1.00 | 1.16 |
| ATOM | 912 | HE3 | MET | 61 | -7.846 | 11.298 | -9.232 | 1.00 | 1.12 |
| ATOM | 913 | C | MET | 61 | -5.396 | 7.540 | -10.524 | 1.00 | 0.20 |
| ATOM | 914 | O | MET | 61 | -5.478 | 6.951 | -9.463 | 1.00 | 0.22 |
| ATOM | 915 | N | ILE | 62 | -4.241 | 7.937 | -11.001 | 1.00 | 0.20 |
| ATOM | 916 | HN | ILE | 62 | -4.207 | 8.393 | -11.868 | 1.00 | 0.21 |
| ATOM | 917 | CA | ILE | 62 | -2.971 | 7.678 | -10.252 | 1.00 | 0.21 |
| ATOM | 918 | HA | ILE | 62 | -3.156 | 6.982 | -9.448 | 1.00 | 0.20 |
| ATOM | 919 | CB | ILE | 62 | -1.938 | 7.080 | -11.211 | 1.00 | 0.24 |
| ATOM | 920 | HB | ILE | 62 | -1.753 | 7.781 | -12.012 | 1.00 | 0.26 |
| ATOM | 921 | CG1 | ILE | 62 | -2.480 | 5.762 | -11.785 | 1.00 | 0.23 |
| ATOM | 922 | HG11 | ILE | 62 | -3.479 | 5.922 | -12.162 | 1.00 | 0.20 |
| ATOM | 923 | HG12 | ILE | 62 | -2.508 | 5.018 | -11.003 | 1.00 | 0.24 |
| ATOM | 924 | CG2 | ILE | 62 | -0.635 | 6.812 | -10.455 | 1.00 | 0.30 |
| ATOM | 925 | HG21 | ILE | 62 | -0.863 | 6.443 | -9.466 | 1.00 | 1.08 |
| ATOM | 926 | HG22 | ILE | 62 | -0.070 | 7.729 | -10.375 | 1.00 | 1.12 |
| ATOM | 927 | HG23 | ILE | 62 | -0.052 | 6.076 | -10.988 | 1.00 | 0.99 |
| ATOM | 928 | CD1 | ILE | 62 | -1.584 | 5.262 | -12.927 | 1.00 | 0.29 |
| ATOM | 929 | HD11 | ILE | 62 | -0.979 | 6.073 | -13.305 | 1.00 | 1.02 |
| ATOM | 930 | HD12 | ILE | 62 | -2.201 | 4.876 | -13.724 | 1.00 | 1.09 |
| ATOM | 931 | HD13 | ILE | 62 | -0.941 | 4.476 | -12.559 | 1.00 | 1.07 |
| ATOM | 932 | C | ILE | 62 | -2.423 | 8.988 | -9.677 | 1.00 | 0.22 |
| ATOM | 933 | O | ILE | 62 | -2.393 | 10.004 | -10.343 | 1.00 | 0.27 |
| ATOM | 934 | N | SER | 63 | -1.993 | 8.976 | -8.441 | 1.00 | 0.20 |
| ATOM | 935 | HN | SER | 63 | -2.028 | 8.147 | -7.916 | 1.00 | 0.18 |
| ATOM | 936 | CA | SER | 63 | -1.452 | 10.226 | -7.829 | 1.00 | 0.22 |
| ATOM | 937 | HA | SER | 63 | -0.998 | 10.836 | -8.597 | 1.00 | 0.26 |
| ATOM | 938 | CB | SER | 63 | -2.597 | 11.000 | -7.176 | 1.00 | 0.24 |
| ATOM | 939 | HB1 | SER | 63 | -3.448 | 11.012 | -7.845 | 1.00 | 0.25 |
| ATOM | 940 | HB2 | SER | 63 | -2.286 | 12.012 | -6.978 | 1.00 | 0.29 |
| ATOM | 941 | OG | SER | 63 | -2.951 | 10.369 | -5.952 | 1.00 | 0.25 |
| ATOM | 942 | HG | SER | 63 | -3.682 | 9.772 | -6.127 | 1.00 | 0.85 |
| ATOM | 943 | C | SER | 63 | -0.404 | 9.879 | -6.764 | 1.00 | 0.21 |
| ATOM | 944 | O | SER | 63 | -0.364 | 8.775 | -6.259 | 1.00 | 0.20 |
| ATOM | 945 | N | PHE | 64 | 0.440 | 10.823 | -6.419 | 1.00 | 0.24 |
| ATOM | 946 | HN | PHE | 64 | 0.380 | 11.705 | -6.841 | 1.00 | 0.27 |
| ATOM | 947 | CA | PHE | 64 | 1.490 | 10.569 | -5.382 | 1.00 | 0.24 |
| ATOM | 948 | HA | PHE | 64 | 1.560 | 9.511 | -5.179 | 1.00 | 0.22 |
| ATOM | 949 | CB | PHE | 64 | 2.840 | 11.084 | -5.895 | 1.00 | 0.28 |
| ATOM | 950 | HB1 | PHE | 64 | 3.564 | 11.047 | -5.097 | 1.00 | 0.32 |
| ATOM | 951 | HB2 | PHE | 64 | 2.730 | 12.103 | -6.235 | 1.00 | 0.32 |
| ATOM | 952 | CG | PHE | 64 | 3.316 | 10.220 | -7.040 | 1.00 | 0.28 |
| ATOM | 953 | CD1 | PHE | 64 | 4.112 | 9.096 | -6.788 | 1.00 | 0.30 |
| ATOM | 954 | HD1 | PHE | 64 | 4.385 | 8.844 | -5.774 | 1.00 | 0.32 |
| ATOM | 955 | CD2 | PHE | 64 | 2.963 | 10.545 | -8.355 | 1.00 | 0.33 |
| ATOM | 956 | HD2 | PHE | 64 | 2.350 | 11.412 | -8.550 | 1.00 | 0.37 |
| ATOM | 957 | CE1 | PHE | 64 | 4.553 | 8.297 | -7.850 | 1.00 | 0.36 |
| ATOM | 958 | HE1 | PHE | 64 | 5.166 | 7.430 | -7.656 | 1.00 | 0.40 |
| ATOM | 959 | CE2 | PHE | 64 | 3.403 | 9.747 | -9.417 | 1.00 | 0.40 |
| ATOM | 960 | HE2 | PHE | 64 | 3.130 | 9.998 | -10.431 | 1.00 | 0.47 |
| ATOM | 961 | CZ | PHE | 64 | 4.198 | 8.623 | -9.165 | 1.00 | 0.40 |
| ATOM | 962 | HZ | PHE | 64 | 4.538 | 8.007 | -9.984 | 1.00 | 0.47 |
| ATOM | 963 | C | PHE | 64 | 1.115 | 11.318 | -4.097 | 1.00 | 0.27 |

17/75

| | | | | | | | | | |
|------|------|------|-----|----|--------|--------|--------|------|------|
| ATOM | 964 | O | PHE | 64 | 0.924 | 12.518 | -4.108 | 1.00 | 0.36 |
| ATOM | 965 | N | GLY | 65 | 0.996 | 10.617 | -2.996 | 1.00 | 0.30 |
| ATOM | 966 | HN | GLY | 65 | 1.146 | 9.649 | -3.017 | 1.00 | 0.33 |
| ATOM | 967 | CA | GLY | 65 | 0.615 | 11.282 | -1.709 | 1.00 | 0.38 |
| ATOM | 968 | HA1 | GLY | 65 | -0.152 | 10.697 | -1.224 | 1.00 | 0.46 |
| ATOM | 969 | HA2 | GLY | 65 | 0.230 | 12.270 | -1.913 | 1.00 | 0.45 |
| ATOM | 970 | C | GLY | 65 | 1.823 | 11.397 | -0.770 | 1.00 | 0.32 |
| ATOM | 971 | O | GLY | 65 | 2.926 | 11.007 | -1.098 | 1.00 | 0.40 |
| ATOM | 972 | N | ILE | 66 | 1.598 | 11.926 | 0.408 | 1.00 | 0.30 |
| ATOM | 973 | HN | ILE | 66 | 0.691 | 12.220 | 0.635 | 1.00 | 0.36 |
| ATOM | 974 | CA | ILE | 66 | 2.691 | 12.081 | 1.417 | 1.00 | 0.36 |
| ATOM | 975 | HA | ILE | 66 | 3.564 | 11.534 | 1.093 | 1.00 | 0.40 |
| ATOM | 976 | CB | ILE | 66 | 3.040 | 13.564 | 1.571 | 1.00 | 0.41 |
| ATOM | 977 | HB | ILE | 66 | 2.127 | 14.134 | 1.656 | 1.00 | 0.64 |
| ATOM | 978 | CG1 | ILE | 66 | 3.829 | 14.026 | 0.337 | 1.00 | 0.68 |
| ATOM | 979 | HG11 | ILE | 66 | 3.301 | 13.729 | -0.557 | 1.00 | 0.95 |
| ATOM | 980 | HG12 | ILE | 66 | 4.804 | 13.561 | 0.346 | 1.00 | 1.01 |
| ATOM | 981 | CG2 | ILE | 66 | 3.886 | 13.764 | 2.831 | 1.00 | 0.93 |
| ATOM | 982 | HG21 | ILE | 66 | 4.372 | 14.727 | 2.790 | 1.00 | 1.50 |
| ATOM | 983 | HG22 | ILE | 66 | 4.632 | 12.986 | 2.891 | 1.00 | 1.41 |
| ATOM | 984 | HG23 | ILE | 66 | 3.249 | 13.720 | 3.702 | 1.00 | 1.54 |
| ATOM | 985 | CD1 | ILE | 66 | 3.997 | 15.551 | 0.343 | 1.00 | 0.70 |
| ATOM | 986 | HD11 | ILE | 66 | 4.944 | 15.806 | 0.797 | 1.00 | 1.22 |
| ATOM | 987 | HD12 | ILE | 66 | 3.196 | 16.009 | 0.902 | 1.00 | 1.28 |
| ATOM | 988 | HD13 | ILE | 66 | 3.979 | 15.917 | -0.673 | 1.00 | 1.23 |
| ATOM | 989 | C | ILE | 66 | 2.207 | 11.519 | 2.760 | 1.00 | 0.46 |
| ATOM | 990 | O | ILE | 66 | 1.021 | 11.363 | 2.958 | 1.00 | 0.54 |
| ATOM | 991 | N | LYS | 67 | 3.129 | 11.205 | 3.659 | 1.00 | 0.59 |
| ATOM | 992 | HN | LYS | 67 | 4.073 | 11.343 | 3.434 | 1.00 | 0.64 |
| ATOM | 993 | CA | LYS | 67 | 2.780 | 10.630 | 5.014 | 1.00 | 0.74 |
| ATOM | 994 | HA | LYS | 67 | 3.072 | 9.594 | 5.038 | 1.00 | 0.83 |
| ATOM | 995 | CB | LYS | 67 | 3.550 | 11.404 | 6.102 | 1.00 | 0.90 |
| ATOM | 996 | HB1 | LYS | 67 | 3.237 | 12.438 | 6.089 | 1.00 | 0.89 |
| ATOM | 997 | HB2 | LYS | 67 | 4.608 | 11.352 | 5.891 | 1.00 | 0.96 |
| ATOM | 998 | CG | LYS | 67 | 3.287 | 10.815 | 7.504 | 1.00 | 1.08 |
| ATOM | 999 | HG1 | LYS | 67 | 2.254 | 10.524 | 7.598 | 1.00 | 1.31 |
| ATOM | 1000 | HG2 | LYS | 67 | 3.510 | 11.565 | 8.249 | 1.00 | 1.33 |
| ATOM | 1001 | CD | LYS | 67 | 4.179 | 9.590 | 7.746 | 1.00 | 0.98 |
| ATOM | 1002 | HD1 | LYS | 67 | 5.216 | 9.885 | 7.694 | 1.00 | 1.07 |
| ATOM | 1003 | HD2 | LYS | 67 | 3.979 | 8.839 | 6.999 | 1.00 | 1.07 |
| ATOM | 1004 | CE | LYS | 67 | 3.885 | 9.016 | 9.135 | 1.00 | 1.17 |
| ATOM | 1005 | HE1 | LYS | 67 | 4.331 | 8.036 | 9.220 | 1.00 | 1.64 |
| ATOM | 1006 | HE2 | LYS | 67 | 2.817 | 8.938 | 9.272 | 1.00 | 1.50 |
| ATOM | 1007 | NZ | LYS | 67 | 4.453 | 9.913 | 10.180 | 1.00 | 1.93 |
| ATOM | 1008 | HZ1 | LYS | 67 | 4.569 | 10.870 | 9.792 | 1.00 | 2.38 |
| ATOM | 1009 | HZ2 | LYS | 67 | 5.378 | 9.547 | 10.485 | 1.00 | 2.43 |
| ATOM | 1010 | HZ3 | LYS | 67 | 3.808 | 9.948 | 10.995 | 1.00 | 2.40 |
| ATOM | 1011 | C | LYS | 67 | 1.274 | 10.732 | 5.280 | 1.00 | 0.72 |
| ATOM | 1012 | O | LYS | 67 | 0.530 | 9.804 | 5.035 | 1.00 | 0.79 |
| ATOM | 1013 | N | GLU | 68 | 0.815 | 11.855 | 5.760 | 1.00 | 0.77 |
| ATOM | 1014 | HN | GLU | 68 | 1.425 | 12.601 | 5.939 | 1.00 | 0.84 |
| ATOM | 1015 | CA | GLU | 68 | -0.645 | 12.004 | 6.011 | 1.00 | 0.84 |
| ATOM | 1016 | HA | GLU | 68 | -1.014 | 11.130 | 6.530 | 1.00 | 0.99 |
| ATOM | 1017 | CB | GLU | 68 | -0.895 | 13.254 | 6.860 | 1.00 | 1.05 |
| ATOM | 1018 | HB1 | GLU | 68 | -0.393 | 13.149 | 7.810 | 1.00 | 1.23 |
| ATOM | 1019 | HB2 | GLU | 68 | -1.956 | 13.370 | 7.024 | 1.00 | 1.10 |
| ATOM | 1020 | CG | GLU | 68 | -0.353 | 14.487 | 6.134 | 1.00 | 1.15 |
| ATOM | 1021 | HG1 | GLU | 68 | -1.000 | 14.730 | 5.304 | 1.00 | 1.32 |
| ATOM | 1022 | HG2 | GLU | 68 | 0.642 | 14.281 | 5.768 | 1.00 | 1.28 |
| ATOM | 1023 | CD | GLU | 68 | -0.308 | 15.669 | 7.104 | 1.00 | 1.75 |
| ATOM | 1024 | OE1 | GLU | 68 | 0.246 | 16.692 | 6.736 | 1.00 | 2.45 |
| ATOM | 1025 | OE2 | GLU | 68 | -0.823 | 15.530 | 8.202 | 1.00 | 2.16 |
| ATOM | 1026 | C | GLU | 68 | -1.346 | 12.132 | 4.660 | 1.00 | 0.76 |
| ATOM | 1027 | O | GLU | 68 | -0.899 | 12.859 | 3.795 | 1.00 | 1.11 |
| ATOM | 1028 | N | HIS | 69 | -2.420 | 11.414 | 4.454 | 1.00 | 0.94 |
| ATOM | 1029 | HN | HIS | 69 | -2.755 | 10.815 | 5.155 | 1.00 | 1.32 |
| ATOM | 1030 | CA | HIS | 69 | -3.114 | 11.487 | 3.136 | 1.00 | 1.04 |
| ATOM | 1031 | HA | HIS | 69 | -2.877 | 12.437 | 2.679 | 1.00 | 1.25 |
| ATOM | 1032 | CB | HIS | 69 | -2.545 | 10.358 | 2.243 | 1.00 | 1.49 |
| ATOM | 1033 | HB1 | HIS | 69 | -1.750 | 9.862 | 2.783 | 1.00 | 2.12 |
| ATOM | 1034 | HB2 | HIS | 69 | -2.131 | 10.798 | 1.351 | 1.00 | 2.27 |
| ATOM | 1035 | CG | HIS | 69 | -3.570 | 9.333 | 1.837 | 1.00 | 0.95 |
| ATOM | 1036 | ND1 | HIS | 69 | -3.818 | 8.195 | 2.588 | 1.00 | 1.43 |
| ATOM | 1037 | HD1 | HIS | 69 | -3.415 | 7.972 | 3.453 | 1.00 | 1.83 |
| ATOM | 1038 | CD2 | HIS | 69 | -4.355 | 9.223 | 0.717 | 1.00 | 1.04 |
| ATOM | 1039 | HD2 | HIS | 69 | -4.403 | 9.946 | -0.082 | 1.00 | 1.41 |
| ATOM | 1040 | CE1 | HIS | 69 | -4.715 | 7.452 | 1.912 | 1.00 | 1.81 |

18/75

| | | | | | | | | | |
|------|------|-----|-----|----|---------|--------|--------|------|------|
| ATOM | 1041 | HE1 | HIS | 69 | -5.097 | 6.502 | 2.257 | 1.00 | 2.54 |
| ATOM | 1042 | NE2 | HIS | 69 | -5.075 | 8.032 | 0.765 | 1.00 | 1.53 |
| ATOM | 1043 | C | HIS | 69 | -4.643 | 11.435 | 3.341 | 1.00 | 1.14 |
| ATOM | 1044 | O | HIS | 69 | -5.392 | 10.889 | 2.556 | 1.00 | 1.76 |
| ATOM | 1045 | N | GLY | 70 | -5.108 | 12.065 | 4.393 | 1.00 | 1.49 |
| ATOM | 1046 | HN | GLY | 70 | -4.487 | 12.532 | 4.990 | 1.00 | 1.98 |
| ATOM | 1047 | CA | GLY | 70 | -6.576 | 12.123 | 4.665 | 1.00 | 1.86 |
| ATOM | 1048 | HA1 | GLY | 70 | -7.071 | 12.633 | 3.852 | 1.00 | 2.28 |
| ATOM | 1049 | HA2 | GLY | 70 | -6.746 | 12.667 | 5.583 | 1.00 | 2.09 |
| ATOM | 1050 | C | GLY | 70 | -7.155 | 10.716 | 4.801 | 1.00 | 1.81 |
| ATOM | 1051 | O | GLY | 70 | -8.182 | 10.404 | 4.232 | 1.00 | 2.53 |
| ATOM | 1052 | N | ASP | 71 | -6.513 | 9.863 | 5.545 | 1.00 | 1.55 |
| ATOM | 1053 | HN | ASP | 71 | -5.686 | 10.127 | 5.999 | 1.00 | 1.66 |
| ATOM | 1054 | CA | ASP | 71 | -7.047 | 8.484 | 5.701 | 1.00 | 1.91 |
| ATOM | 1055 | HA | ASP | 71 | -8.126 | 8.513 | 5.684 | 1.00 | 2.42 |
| ATOM | 1056 | CB | ASP | 71 | -6.546 | 7.620 | 4.546 | 1.00 | 2.67 |
| ATOM | 1057 | HB1 | ASP | 71 | -6.623 | 6.578 | 4.813 | 1.00 | 3.03 |
| ATOM | 1058 | HB2 | ASP | 71 | -5.514 | 7.865 | 4.341 | 1.00 | 2.88 |
| ATOM | 1059 | CG | ASP | 71 | -7.397 | 7.892 | 3.303 | 1.00 | 3.56 |
| ATOM | 1060 | OD1 | ASP | 71 | -8.476 | 7.330 | 3.215 | 1.00 | 4.08 |
| ATOM | 1061 | OD2 | ASP | 71 | -6.960 | 8.664 | 2.465 | 1.00 | 4.16 |
| ATOM | 1062 | C | ASP | 71 | -6.577 | 7.889 | 7.028 | 1.00 | 1.46 |
| ATOM | 1063 | O | ASP | 71 | -5.600 | 8.323 | 7.605 | 1.00 | 1.78 |
| ATOM | 1064 | N | PHE | 72 | -7.260 | 6.886 | 7.507 | 1.00 | 1.36 |
| ATOM | 1065 | HN | PHE | 72 | -8.038 | 6.546 | 7.018 | 1.00 | 1.67 |
| ATOM | 1066 | CA | PHE | 72 | -6.849 | 6.248 | 8.786 | 1.00 | 1.48 |
| ATOM | 1067 | HA | PHE | 72 | -6.504 | 7.007 | 9.473 | 1.00 | 1.75 |
| ATOM | 1068 | CB | PHE | 72 | -8.037 | 5.503 | 9.399 | 1.00 | 2.01 |
| ATOM | 1069 | HB1 | PHE | 72 | -8.374 | 6.028 | 10.281 | 1.00 | 2.58 |
| ATOM | 1070 | HB2 | PHE | 72 | -7.733 | 4.503 | 9.669 | 1.00 | 2.43 |
| ATOM | 1071 | CG | PHE | 72 | -9.161 | 5.434 | 8.395 | 1.00 | 2.30 |
| ATOM | 1072 | CD1 | PHE | 72 | -9.414 | 4.243 | 7.704 | 1.00 | 2.86 |
| ATOM | 1073 | HD1 | PHE | 72 | -8.802 | 3.372 | 7.887 | 1.00 | 3.09 |
| ATOM | 1074 | CD2 | PHE | 72 | -9.954 | 6.563 | 8.158 | 1.00 | 2.97 |
| ATOM | 1075 | HD2 | PHE | 72 | -9.758 | 7.482 | 8.691 | 1.00 | 3.28 |
| ATOM | 1076 | CE1 | PHE | 72 | -10.459 | 4.182 | 6.775 | 1.00 | 3.73 |
| ATOM | 1077 | HE1 | PHE | 72 | -10.655 | 3.264 | 6.242 | 1.00 | 4.46 |
| ATOM | 1078 | CE2 | PHE | 72 | -10.999 | 6.502 | 7.229 | 1.00 | 3.80 |
| ATOM | 1079 | HE2 | PHE | 72 | -11.610 | 7.374 | 7.045 | 1.00 | 4.54 |
| ATOM | 1080 | CZ | PHE | 72 | -11.252 | 5.312 | 6.537 | 1.00 | 4.08 |
| ATOM | 1081 | HZ | PHE | 72 | -12.058 | 5.264 | 5.821 | 1.00 | 4.92 |
| ATOM | 1082 | C | PHE | 72 | -5.716 | 5.266 | 8.500 | 1.00 | 1.41 |
| ATOM | 1083 | O | PHE | 72 | -5.384 | 4.430 | 9.318 | 1.00 | 2.20 |
| ATOM | 1084 | N | TYR | 73 | -5.120 | 5.371 | 7.338 | 1.00 | 1.12 |
| ATOM | 1085 | HN | TYR | 73 | -5.412 | 6.059 | 6.703 | 1.00 | 1.48 |
| ATOM | 1086 | CA | TYR | 73 | -3.999 | 4.457 | 6.972 | 1.00 | 1.25 |
| ATOM | 1087 | HA | TYR | 73 | -3.774 | 3.793 | 7.790 | 1.00 | 1.46 |
| ATOM | 1088 | CB | TYR | 73 | -4.391 | 3.635 | 5.742 | 1.00 | 1.86 |
| ATOM | 1089 | HB1 | TYR | 73 | -3.531 | 3.082 | 5.395 | 1.00 | 2.35 |
| ATOM | 1090 | HB2 | TYR | 73 | -4.726 | 4.300 | 4.961 | 1.00 | 2.46 |
| ATOM | 1091 | CG | TYR | 73 | -5.498 | 2.670 | 6.089 | 1.00 | 2.08 |
| ATOM | 1092 | CD1 | TYR | 73 | -5.241 | 1.585 | 6.934 | 1.00 | 2.58 |
| ATOM | 1093 | HD1 | TYR | 73 | -4.252 | 1.444 | 7.347 | 1.00 | 2.82 |
| ATOM | 1094 | CD2 | TYR | 73 | -6.779 | 2.853 | 5.553 | 1.00 | 2.85 |
| ATOM | 1095 | HD2 | TYR | 73 | -6.978 | 3.691 | 4.901 | 1.00 | 3.24 |
| ATOM | 1096 | CE1 | TYR | 73 | -6.264 | 0.683 | 7.244 | 1.00 | 3.48 |
| ATOM | 1097 | HE1 | TYR | 73 | -6.066 | -0.155 | 7.896 | 1.00 | 4.19 |
| ATOM | 1098 | CE2 | TYR | 73 | -7.802 | 1.952 | 5.865 | 1.00 | 3.68 |
| ATOM | 1099 | HE2 | TYR | 73 | -8.789 | 2.093 | 5.452 | 1.00 | 4.49 |
| ATOM | 1100 | CZ | TYR | 73 | -7.545 | 0.866 | 6.710 | 1.00 | 3.90 |
| ATOM | 1101 | OH | TYR | 73 | -8.554 | -0.024 | 7.013 | 1.00 | 5.00 |
| ATOM | 1102 | HH | TYR | 73 | -8.689 | -0.590 | 6.249 | 1.00 | 5.22 |
| ATOM | 1103 | C | TYR | 73 | -2.755 | 5.273 | 6.609 | 1.00 | 0.95 |
| ATOM | 1104 | O | TYR | 73 | -2.219 | 5.127 | 5.529 | 1.00 | 1.21 |
| ATOM | 1105 | N | PRO | 74 | -2.273 | 6.106 | 7.495 | 1.00 | 0.74 |
| ATOM | 1106 | CA | PRO | 74 | -1.054 | 6.895 | 7.197 | 1.00 | 0.82 |
| ATOM | 1107 | HA | PRO | 74 | -1.254 | 7.648 | 6.453 | 1.00 | 1.05 |
| ATOM | 1108 | CB | PRO | 74 | -0.746 | 7.558 | 8.543 | 1.00 | 1.18 |
| ATOM | 1109 | HB1 | PRO | 74 | -0.786 | 8.631 | 8.438 | 1.00 | 1.46 |
| ATOM | 1110 | HB2 | PRO | 74 | 0.239 | 7.261 | 8.876 | 1.00 | 1.28 |
| ATOM | 1111 | CG | PRO | 74 | -1.795 | 7.105 | 9.566 | 1.00 | 1.35 |
| ATOM | 1112 | HG1 | PRO | 74 | -2.229 | 7.967 | 10.049 | 1.00 | 1.70 |
| ATOM | 1113 | HG2 | PRO | 74 | -1.330 | 6.468 | 10.305 | 1.00 | 1.61 |
| ATOM | 1114 | CD | PRO | 74 | -2.889 | 6.328 | 8.828 | 1.00 | 1.04 |
| ATOM | 1115 | HD2 | PRO | 74 | -3.098 | 5.393 | 9.328 | 1.00 | 1.24 |
| ATOM | 1116 | HD1 | PRO | 74 | -3.778 | 6.929 | 8.733 | 1.00 | 1.14 |
| ATOM | 1117 | C | PRO | 74 | 0.097 | 5.988 | 6.765 | 1.00 | 0.65 |

19/75

| | | | | | | | | | |
|------|------|-----|-----|----|--------|--------|-------|------|------|
| ATOM | 1118 | O | PRO | 74 | 0.136 | 4.822 | 7.106 | 1.00 | 0.66 |
| ATOM | 1119 | N | PHE | 75 | 1.038 | 6.503 | 6.032 | 1.00 | 0.56 |
| ATOM | 1120 | HN | PHE | 75 | 1.000 | 7.447 | 5.770 | 1.00 | 0.61 |
| ATOM | 1121 | CA | PHE | 75 | 2.179 | 5.651 | 5.605 | 1.00 | 0.45 |
| ATOM | 1122 | HA | PHE | 75 | 1.816 | 4.659 | 5.360 | 1.00 | 0.48 |
| ATOM | 1123 | CB | PHE | 75 | 2.859 | 6.266 | 4.379 | 1.00 | 0.42 |
| ATOM | 1124 | HB1 | PHE | 75 | 3.761 | 5.718 | 4.153 | 1.00 | 0.44 |
| ATOM | 1125 | HB2 | PHE | 75 | 3.104 | 7.298 | 4.582 | 1.00 | 0.45 |
| ATOM | 1126 | CG | PHE | 75 | 1.915 | 6.190 | 3.200 | 1.00 | 0.48 |
| ATOM | 1127 | CD1 | PHE | 75 | 1.764 | 4.986 | 2.501 | 1.00 | 0.41 |
| ATOM | 1128 | HD1 | PHE | 75 | 2.329 | 4.115 | 2.797 | 1.00 | 0.45 |
| ATOM | 1129 | CD2 | PHE | 75 | 1.184 | 7.320 | 2.812 | 1.00 | 0.74 |
| ATOM | 1130 | HD2 | PHE | 75 | 1.300 | 8.249 | 3.349 | 1.00 | 0.90 |
| ATOM | 1131 | CE1 | PHE | 75 | 0.882 | 4.911 | 1.415 | 1.00 | 0.50 |
| ATOM | 1132 | HE1 | PHE | 75 | 0.767 | 3.982 | 0.877 | 1.00 | 0.53 |
| ATOM | 1133 | CE2 | PHE | 75 | 0.304 | 7.245 | 1.724 | 1.00 | 0.85 |
| ATOM | 1134 | HE2 | PHE | 75 | -0.258 | 8.117 | 1.423 | 1.00 | 1.09 |
| ATOM | 1135 | CZ | PHE | 75 | 0.154 | 6.041 | 1.026 | 1.00 | 0.69 |
| ATOM | 1136 | HZ | PHE | 75 | -0.526 | 5.983 | 0.188 | 1.00 | 0.80 |
| ATOM | 1137 | C | PHE | 75 | 3.159 | 5.561 | 6.776 | 1.00 | 0.43 |
| ATOM | 1138 | O | PHE | 75 | 3.111 | 6.360 | 7.690 | 1.00 | 0.50 |
| ATOM | 1139 | N | ASP | 76 | 4.020 | 4.582 | 6.782 | 1.00 | 0.37 |
| ATOM | 1140 | HN | ASP | 76 | 4.028 | 3.929 | 6.050 | 1.00 | 0.32 |
| ATOM | 1141 | CA | ASP | 76 | 4.967 | 4.432 | 7.927 | 1.00 | 0.43 |
| ATOM | 1142 | HA | ASP | 76 | 4.551 | 4.906 | 8.804 | 1.00 | 0.50 |
| ATOM | 1143 | CB | ASP | 76 | 5.180 | 2.946 | 8.215 | 1.00 | 0.46 |
| ATOM | 1144 | HB1 | ASP | 76 | 4.224 | 2.467 | 8.365 | 1.00 | 0.49 |
| ATOM | 1145 | HB2 | ASP | 76 | 5.784 | 2.834 | 9.104 | 1.00 | 0.54 |
| ATOM | 1146 | CG | ASP | 76 | 5.892 | 2.295 | 7.028 | 1.00 | 0.38 |
| ATOM | 1147 | OD1 | ASP | 76 | 6.468 | 1.236 | 7.218 | 1.00 | 0.45 |
| ATOM | 1148 | OD2 | ASP | 76 | 5.846 | 2.864 | 5.950 | 1.00 | 0.30 |
| ATOM | 1149 | C | ASP | 76 | 6.314 | 5.074 | 7.596 | 1.00 | 0.42 |
| ATOM | 1150 | O | ASP | 76 | 7.314 | 4.770 | 8.216 | 1.00 | 0.54 |
| ATOM | 1151 | N | GLY | 77 | 6.347 | 5.958 | 6.632 | 1.00 | 0.35 |
| ATOM | 1152 | HN | GLY | 77 | 5.525 | 6.187 | 6.151 | 1.00 | 0.36 |
| ATOM | 1153 | CA | GLY | 77 | 7.634 | 6.625 | 6.267 | 1.00 | 0.38 |
| ATOM | 1154 | HA1 | GLY | 77 | 8.378 | 6.388 | 7.004 | 1.00 | 0.45 |
| ATOM | 1155 | HA2 | GLY | 77 | 7.484 | 7.696 | 6.238 | 1.00 | 0.44 |
| ATOM | 1156 | C | GLY | 77 | 8.084 | 6.131 | 4.884 | 1.00 | 0.31 |
| ATOM | 1157 | O | GLY | 77 | 7.262 | 5.767 | 4.068 | 1.00 | 0.37 |
| ATOM | 1158 | N | PRO | 78 | 9.370 | 6.117 | 4.603 | 1.00 | 0.33 |
| ATOM | 1159 | CA | PRO | 78 | 9.856 | 5.651 | 3.274 | 1.00 | 0.36 |
| ATOM | 1160 | HA | PRO | 78 | 9.435 | 6.254 | 2.488 | 1.00 | 0.42 |
| ATOM | 1161 | CB | PRO | 78 | 11.364 | 5.903 | 3.359 | 1.00 | 0.46 |
| ATOM | 1162 | HB1 | PRO | 78 | 11.671 | 6.542 | 2.545 | 1.00 | 0.56 |
| ATOM | 1163 | HB2 | PRO | 78 | 11.892 | 4.962 | 3.303 | 1.00 | 0.48 |
| ATOM | 1164 | CG | PRO | 78 | 11.675 | 6.592 | 4.694 | 1.00 | 0.64 |
| ATOM | 1165 | HG1 | PRO | 78 | 11.965 | 7.616 | 4.516 | 1.00 | 0.87 |
| ATOM | 1166 | HG2 | PRO | 78 | 12.478 | 6.068 | 5.194 | 1.00 | 0.83 |
| ATOM | 1167 | CD | PRO | 78 | 10.418 | 6.562 | 5.563 | 1.00 | 0.45 |
| ATOM | 1168 | HD2 | PRO | 78 | 10.535 | 5.848 | 6.369 | 1.00 | 0.48 |
| ATOM | 1169 | HD1 | PRO | 78 | 10.187 | 7.544 | 5.944 | 1.00 | 0.49 |
| ATOM | 1170 | C | PRO | 78 | 9.564 | 4.165 | 3.027 | 1.00 | 0.30 |
| ATOM | 1171 | O | PRO | 78 | 8.860 | 3.808 | 2.105 | 1.00 | 0.28 |
| ATOM | 1172 | N | SER | 79 | 10.102 | 3.297 | 3.840 | 1.00 | 0.31 |
| ATOM | 1173 | HN | SER | 79 | 10.670 | 3.604 | 4.577 | 1.00 | 0.35 |
| ATOM | 1174 | CA | SER | 79 | 9.855 | 1.837 | 3.647 | 1.00 | 0.30 |
| ATOM | 1175 | HA | SER | 79 | 9.916 | 1.599 | 2.595 | 1.00 | 0.30 |
| ATOM | 1176 | CB | SER | 79 | 10.911 | 1.037 | 4.410 | 1.00 | 0.37 |
| ATOM | 1177 | HB1 | SER | 79 | 11.888 | 1.465 | 4.225 | 1.00 | 0.42 |
| ATOM | 1178 | HB2 | SER | 79 | 10.901 | 0.013 | 4.076 | 1.00 | 0.39 |
| ATOM | 1179 | OG | SER | 79 | 10.617 | 1.080 | 5.800 | 1.00 | 0.38 |
| ATOM | 1180 | HG | SER | 79 | 11.173 | 1.752 | 6.201 | 1.00 | 0.98 |
| ATOM | 1181 | C | SER | 79 | 8.463 | 1.470 | 4.173 | 1.00 | 0.27 |
| ATOM | 1182 | O | SER | 79 | 7.888 | 2.183 | 4.971 | 1.00 | 0.25 |
| ATOM | 1183 | N | GLY | 80 | 7.927 | 0.356 | 3.734 | 1.00 | 0.31 |
| ATOM | 1184 | HN | GLY | 80 | 8.420 | -0.200 | 3.095 | 1.00 | 0.37 |
| ATOM | 1185 | CA | GLY | 80 | 6.576 | -0.081 | 4.207 | 1.00 | 0.30 |
| ATOM | 1186 | HA1 | GLY | 80 | 6.224 | 0.586 | 4.977 | 1.00 | 0.31 |
| ATOM | 1187 | HA2 | GLY | 80 | 6.646 | -1.083 | 4.607 | 1.00 | 0.36 |
| ATOM | 1188 | C | GLY | 80 | 5.584 | -0.070 | 3.042 | 1.00 | 0.25 |
| ATOM | 1189 | O | GLY | 80 | 5.850 | -0.601 | 1.981 | 1.00 | 0.25 |
| ATOM | 1190 | N | LEU | 81 | 4.440 | 0.531 | 3.232 | 1.00 | 0.23 |
| ATOM | 1191 | HN | LEU | 81 | 4.246 | 0.951 | 4.096 | 1.00 | 0.25 |
| ATOM | 1192 | CA | LEU | 81 | 3.428 | 0.577 | 2.138 | 1.00 | 0.21 |
| ATOM | 1193 | HA | LEU | 81 | 3.259 | -0.417 | 1.761 | 1.00 | 0.22 |
| ATOM | 1194 | CB | LEU | 81 | 2.123 | 1.164 | 2.692 | 1.00 | 0.24 |

20/75

| | | | | | | | | | |
|------|------|------|-----|----|---------|--------|--------|------|------|
| ATOM | 1195 | HB1 | LEU | 81 | 1.587 | 1.658 | 1.896 | 1.00 | 0.25 |
| ATOM | 1196 | HB2 | LEU | 81 | 2.356 | 1.881 | 3.465 | 1.00 | 0.29 |
| ATOM | 1197 | CG | LEU | 81 | 1.240 | 0.058 | 3.283 | 1.00 | 0.28 |
| ATOM | 1198 | HG | LEU | 81 | 1.856 | -0.678 | 3.779 | 1.00 | 0.31 |
| ATOM | 1199 | CD1 | LEU | 81 | 0.265 | 0.680 | 4.285 | 1.00 | 0.33 |
| ATOM | 1200 | HD11 | LEU | 81 | 0.071 | 1.706 | 4.009 | 1.00 | 1.05 |
| ATOM | 1201 | HD12 | LEU | 81 | 0.696 | 0.649 | 5.274 | 1.00 | 1.10 |
| ATOM | 1202 | HD13 | LEU | 81 | -0.662 | 0.125 | 4.278 | 1.00 | 1.06 |
| ATOM | 1203 | CD2 | LEU | 81 | 0.426 | -0.606 | 2.168 | 1.00 | 0.31 |
| ATOM | 1204 | HD21 | LEU | 81 | 1.087 | -0.997 | 1.412 | 1.00 | 1.02 |
| ATOM | 1205 | HD22 | LEU | 81 | -0.233 | 0.126 | 1.724 | 1.00 | 1.09 |
| ATOM | 1206 | HD23 | LEU | 81 | -0.161 | -1.411 | 2.584 | 1.00 | 1.06 |
| ATOM | 1207 | C | LEU | 81 | 3.953 | 1.475 | 1.017 | 1.00 | 0.20 |
| ATOM | 1208 | O | LEU | 81 | 3.988 | 2.679 | 1.141 | 1.00 | 0.22 |
| ATOM | 1209 | N | LEU | 82 | 4.366 | 0.899 | -0.078 | 1.00 | 0.18 |
| ATOM | 1210 | HN | LEU | 82 | 4.334 | -0.077 | -0.162 | 1.00 | 0.18 |
| ATOM | 1211 | CA | LEU | 82 | 4.901 | 1.728 | -1.195 | 1.00 | 0.18 |
| ATOM | 1212 | HA | LEU | 82 | 5.519 | 2.520 | -0.799 | 1.00 | 0.19 |
| ATOM | 1213 | CB | LEU | 82 | 5.728 | 0.840 | -2.128 | 1.00 | 0.18 |
| ATOM | 1214 | HB1 | LEU | 82 | 6.235 | 1.457 | -2.854 | 1.00 | 0.20 |
| ATOM | 1215 | HB2 | LEU | 82 | 5.071 | 0.151 | -2.640 | 1.00 | 0.20 |
| ATOM | 1216 | CG | LEU | 82 | 6.763 | 0.050 | -1.323 | 1.00 | 0.18 |
| ATOM | 1217 | HG | LEU | 82 | 6.262 | -0.523 | -0.556 | 1.00 | 0.22 |
| ATOM | 1218 | CD1 | LEU | 82 | 7.513 | -0.898 | -2.259 | 1.00 | 0.17 |
| ATOM | 1219 | HD11 | LEU | 82 | 8.102 | -0.321 | -2.957 | 1.00 | 0.97 |
| ATOM | 1220 | HD12 | LEU | 82 | 6.802 | -1.503 | -2.802 | 1.00 | 0.95 |
| ATOM | 1221 | HD13 | LEU | 82 | 8.163 | -1.537 | -1.681 | 1.00 | 0.98 |
| ATOM | 1222 | CD2 | LEU | 82 | 7.764 | 1.010 | -0.675 | 1.00 | 0.23 |
| ATOM | 1223 | HD21 | LEU | 82 | 8.019 | 1.790 | -1.375 | 1.00 | 1.03 |
| ATOM | 1224 | HD22 | LEU | 82 | 8.657 | 0.466 | -0.403 | 1.00 | 1.07 |
| ATOM | 1225 | HD23 | LEU | 82 | 7.326 | 1.447 | 0.209 | 1.00 | 1.02 |
| ATOM | 1226 | C | LEU | 82 | 3.740 | 2.329 | -1.986 | 1.00 | 0.19 |
| ATOM | 1227 | O | LEU | 82 | 3.882 | 3.341 | -2.646 | 1.00 | 0.21 |
| ATOM | 1228 | N | ALA | 83 | 2.594 | 1.711 | -1.919 | 1.00 | 0.21 |
| ATOM | 1229 | HN | ALA | 83 | 2.512 | 0.899 | -1.376 | 1.00 | 0.24 |
| ATOM | 1230 | CA | ALA | 83 | 1.410 | 2.225 | -2.662 | 1.00 | 0.22 |
| ATOM | 1231 | HA | ALA | 83 | 1.217 | 3.251 | -2.381 | 1.00 | 0.22 |
| ATOM | 1232 | CB | ALA | 83 | 1.668 | 2.140 | -4.171 | 1.00 | 0.23 |
| ATOM | 1233 | HB1 | ALA | 83 | 2.522 | 2.746 | -4.429 | 1.00 | 0.98 |
| ATOM | 1234 | HB2 | ALA | 83 | 0.801 | 2.497 | -4.705 | 1.00 | 1.00 |
| ATOM | 1235 | HB3 | ALA | 83 | 1.860 | 1.113 | -4.445 | 1.00 | 1.05 |
| ATOM | 1236 | C | ALA | 83 | 0.204 | 1.350 | -2.317 | 1.00 | 0.27 |
| ATOM | 1237 | O | ALA | 83 | 0.342 | 0.301 | -1.720 | 1.00 | 0.36 |
| ATOM | 1238 | N | HIS | 84 | -0.976 | 1.762 | -2.686 | 1.00 | 0.24 |
| ATOM | 1239 | HN | HIS | 84 | -1.075 | 2.609 | -3.170 | 1.00 | 0.20 |
| ATOM | 1240 | CA | HIS | 84 | -2.173 | 0.933 | -2.370 | 1.00 | 0.30 |
| ATOM | 1241 | HA | HIS | 84 | -1.940 | -0.108 | -2.542 | 1.00 | 0.36 |
| ATOM | 1242 | CB | HIS | 84 | -2.562 | 1.127 | -0.903 | 1.00 | 0.40 |
| ATOM | 1243 | HB1 | HIS | 84 | -1.695 | 0.965 | -0.278 | 1.00 | 0.48 |
| ATOM | 1244 | HB2 | HIS | 84 | -3.332 | 0.419 | -0.638 | 1.00 | 0.45 |
| ATOM | 1245 | CG | HIS | 84 | -3.074 | 2.525 | -0.692 | 1.00 | 0.44 |
| ATOM | 1246 | ND1 | HIS | 84 | -4.384 | 2.781 | -0.321 | 1.00 | 1.32 |
| ATOM | 1247 | HD1 | HIS | 84 | -5.084 | 2.112 | -0.169 | 1.00 | 2.02 |
| ATOM | 1248 | CD2 | HIS | 84 | -2.465 | 3.752 | -0.788 | 1.00 | 0.74 |
| ATOM | 1249 | HD2 | HIS | 84 | -1.432 | 3.915 | -1.060 | 1.00 | 1.58 |
| ATOM | 1250 | CE1 | HIS | 84 | -4.521 | 4.114 | -0.208 | 1.00 | 1.21 |
| ATOM | 1251 | HE1 | HIS | 84 | -5.441 | 4.606 | 0.071 | 1.00 | 1.87 |
| ATOM | 1252 | NE2 | HIS | 84 | -3.381 | 4.754 | -0.482 | 1.00 | 0.53 |
| ATOM | 1253 | C | HIS | 84 | -3.337 | 1.343 | -3.274 | 1.00 | 0.25 |
| ATOM | 1254 | O | HIS | 84 | -3.347 | 2.417 | -3.843 | 1.00 | 0.23 |
| ATOM | 1255 | N | ALA | 85 | -4.313 | 0.489 | -3.417 | 1.00 | 0.27 |
| ATOM | 1256 | HN | ALA | 85 | -4.279 | -0.374 | -2.954 | 1.00 | 0.34 |
| ATOM | 1257 | CA | ALA | 85 | -5.474 | 0.817 | -4.291 | 1.00 | 0.24 |
| ATOM | 1258 | HA | ALA | 85 | -5.582 | 1.890 | -4.364 | 1.00 | 0.22 |
| ATOM | 1259 | CB | ALA | 85 | -5.236 | 0.231 | -5.685 | 1.00 | 0.25 |
| ATOM | 1260 | HB1 | ALA | 85 | -5.079 | -0.835 | -5.605 | 1.00 | 1.05 |
| ATOM | 1261 | HB2 | ALA | 85 | -4.364 | 0.690 | -6.126 | 1.00 | 1.05 |
| ATOM | 1262 | HB3 | ALA | 85 | -6.097 | 0.420 | -6.308 | 1.00 | 1.06 |
| ATOM | 1263 | C | ALA | 85 | -6.748 | 0.210 | -3.698 | 1.00 | 0.26 |
| ATOM | 1264 | O | ALA | 85 | -6.694 | -0.611 | -2.804 | 1.00 | 0.33 |
| ATOM | 1265 | N | PHE | 86 | -7.892 | 0.605 | -4.198 | 1.00 | 0.28 |
| ATOM | 1266 | HN | PHE | 86 | -7.905 | 1.264 | -4.922 | 1.00 | 0.31 |
| ATOM | 1267 | CA | PHE | 86 | -9.179 | 0.053 | -3.677 | 1.00 | 0.34 |
| ATOM | 1268 | HA | PHE | 86 | -9.000 | -0.443 | -2.737 | 1.00 | 0.39 |
| ATOM | 1269 | CB | PHE | 86 | -10.170 | 1.205 | -3.471 | 1.00 | 0.36 |
| ATOM | 1270 | HB1 | PHE | 86 | -11.177 | 0.821 | -3.459 | 1.00 | 0.42 |
| ATOM | 1271 | HB2 | PHE | 86 | -10.068 | 1.913 | -4.279 | 1.00 | 0.33 |

21/75

| | | | | | | | | | |
|------|------|------|-----|----|---------|--------|---------|------|------|
| ATOM | 1272 | CG | PHE | 86 | -9.877 | 1.896 | -2.159 | 1.00 | 0.39 |
| ATOM | 1273 | CD1 | PHE | 86 | -8.784 | 2.764 | -2.050 | 1.00 | 0.46 |
| ATOM | 1274 | HD1 | PHE | 86 | -8.146 | 2.939 | -2.903 | 1.00 | 0.67 |
| ATOM | 1275 | CD2 | PHE | 86 | -10.703 | 1.670 | -1.051 | 1.00 | 0.67 |
| ATOM | 1276 | HD2 | PHE | 86 | -11.546 | 1.001 | -1.133 | 1.00 | 0.91 |
| ATOM | 1277 | CE1 | PHE | 86 | -8.516 | 3.406 | -0.835 | 1.00 | 0.50 |
| ATOM | 1278 | HE1 | PHE | 86 | -7.673 | 4.075 | -0.751 | 1.00 | 0.69 |
| ATOM | 1279 | CE2 | PHE | 86 | -10.435 | 2.311 | 0.165 | 1.00 | 0.74 |
| ATOM | 1280 | HE2 | PHE | 86 | -11.071 | 2.136 | 1.020 | 1.00 | 1.02 |
| ATOM | 1281 | CZ | PHE | 86 | -9.342 | 3.179 | 0.273 | 1.00 | 0.54 |
| ATOM | 1282 | HZ | PHE | 86 | -9.135 | 3.674 | 1.211 | 1.00 | 0.62 |
| ATOM | 1283 | C | PHE | 86 | -9.746 | -0.940 | -4.710 | 1.00 | 0.36 |
| ATOM | 1284 | O | PHE | 86 | -9.480 | -0.812 | -5.889 | 1.00 | 0.34 |
| ATOM | 1285 | N | PRO | 87 | -10.516 | -1.926 | -4.293 | 1.00 | 0.43 |
| ATOM | 1286 | CA | PRO | 87 | -11.082 | -2.914 | -5.257 | 1.00 | 0.46 |
| ATOM | 1287 | HA | PRO | 87 | -10.296 | -3.524 | -5.665 | 1.00 | 0.53 |
| ATOM | 1288 | CB | PRO | 87 | -11.990 | -3.770 | -4.370 | 1.00 | 0.60 |
| ATOM | 1289 | HB1 | PRO | 87 | -11.644 | -4.792 | -4.377 | 1.00 | 0.69 |
| ATOM | 1290 | HB2 | PRO | 87 | -13.004 | -3.727 | -4.742 | 1.00 | 0.73 |
| ATOM | 1291 | CG | PRO | 87 | -11.943 | -3.225 | -2.937 | 1.00 | 0.58 |
| ATOM | 1292 | HG1 | PRO | 87 | -11.694 | -4.022 | -2.253 | 1.00 | 0.61 |
| ATOM | 1293 | HG2 | PRO | 87 | -12.905 | -2.808 | -2.676 | 1.00 | 0.66 |
| ATOM | 1294 | CD | PRO | 87 | -10.872 | -2.135 | -2.861 | 1.00 | 0.50 |
| ATOM | 1295 | HD2 | PRO | 87 | -11.277 | -1.235 | -2.421 | 1.00 | 0.50 |
| ATOM | 1296 | HD1 | PRO | 87 | -10.014 | -2.484 | -2.309 | 1.00 | 0.52 |
| ATOM | 1297 | C | PRO | 87 | -11.895 | -2.246 | -6.379 | 1.00 | 0.40 |
| ATOM | 1298 | O | PRO | 87 | -12.221 | -1.078 | -6.299 | 1.00 | 0.42 |
| ATOM | 1299 | N | PRO | 88 | -12.221 | -2.981 | -7.419 | 1.00 | 0.44 |
| ATOM | 1300 | CA | PRO | 88 | -13.007 | -2.416 | -8.554 | 1.00 | 0.48 |
| ATOM | 1301 | HA | PRO | 88 | -12.443 | -1.645 | -9.053 | 1.00 | 0.52 |
| ATOM | 1302 | CB | PRO | 88 | -13.163 | -3.622 | -9.488 | 1.00 | 0.61 |
| ATOM | 1303 | HB1 | PRO | 88 | -12.604 | -3.449 | -10.395 | 1.00 | 0.83 |
| ATOM | 1304 | HB2 | PRO | 88 | -14.204 | -3.772 | -9.728 | 1.00 | 0.74 |
| ATOM | 1305 | CG | PRO | 88 | -12.609 | -4.863 | -8.781 | 1.00 | 0.57 |
| ATOM | 1306 | HG1 | PRO | 88 | -11.945 | -5.395 | -9.446 | 1.00 | 0.71 |
| ATOM | 1307 | HG2 | PRO | 88 | -13.425 | -5.508 | -8.488 | 1.00 | 0.64 |
| ATOM | 1308 | CD | PRO | 88 | -11.835 | -4.413 | -7.540 | 1.00 | 0.56 |
| ATOM | 1309 | HD2 | PRO | 88 | -12.146 | -4.977 | -6.671 | 1.00 | 0.62 |
| ATOM | 1310 | HD1 | PRO | 88 | -10.773 | -4.503 | -7.702 | 1.00 | 0.65 |
| ATOM | 1311 | C | PRO | 88 | -14.372 | -1.873 | -8.109 | 1.00 | 0.47 |
| ATOM | 1312 | O | PRO | 88 | -15.380 | -2.551 | -8.172 | 1.00 | 0.88 |
| ATOM | 1313 | N | GLY | 89 | -14.400 | -0.647 | -7.661 | 1.00 | 0.63 |
| ATOM | 1314 | HN | GLY | 89 | -13.571 | -0.129 | -7.626 | 1.00 | 1.01 |
| ATOM | 1315 | CA | GLY | 89 | -15.681 | -0.026 | -7.209 | 1.00 | 0.65 |
| ATOM | 1316 | HA1 | GLY | 89 | -15.536 | 0.422 | -6.239 | 1.00 | 0.62 |
| ATOM | 1317 | HA2 | GLY | 89 | -16.455 | -0.778 | -7.148 | 1.00 | 0.78 |
| ATOM | 1318 | C | GLY | 89 | -16.092 | 1.057 | -8.210 | 1.00 | 0.74 |
| ATOM | 1319 | O | GLY | 89 | -15.541 | 1.151 | -9.289 | 1.00 | 0.84 |
| ATOM | 1320 | N | PRO | 90 | -17.044 | 1.878 | -7.852 | 1.00 | 0.95 |
| ATOM | 1321 | CA | PRO | 90 | -17.499 | 2.973 | -8.750 | 1.00 | 1.19 |
| ATOM | 1322 | HA | PRO | 90 | -17.819 | 2.565 | -9.697 | 1.00 | 1.37 |
| ATOM | 1323 | CB | PRO | 90 | -18.720 | 3.532 | -7.990 | 1.00 | 1.55 |
| ATOM | 1324 | HB1 | PRO | 90 | -19.602 | 3.432 | -8.605 | 1.00 | 1.85 |
| ATOM | 1325 | HB2 | PRO | 90 | -18.572 | 4.567 | -7.740 | 1.00 | 1.74 |
| ATOM | 1326 | CG | PRO | 90 | -18.913 | 2.724 | -6.702 | 1.00 | 1.46 |
| ATOM | 1327 | HG1 | PRO | 90 | -19.828 | 2.155 | -6.763 | 1.00 | 1.60 |
| ATOM | 1328 | HG2 | PRO | 90 | -18.959 | 3.396 | -5.857 | 1.00 | 1.57 |
| ATOM | 1329 | CD | PRO | 90 | -17.729 | 1.769 | -6.539 | 1.00 | 1.17 |
| ATOM | 1330 | HD2 | PRO | 90 | -17.083 | 2.099 | -5.736 | 1.00 | 1.17 |
| ATOM | 1331 | HD1 | PRO | 90 | -18.067 | 0.759 | -6.375 | 1.00 | 1.28 |
| ATOM | 1332 | C | PRO | 90 | -16.375 | 4.011 | -8.972 | 1.00 | 1.14 |
| ATOM | 1333 | O | PRO | 90 | -15.269 | 3.649 | -9.320 | 1.00 | 1.53 |
| ATOM | 1334 | N | ASN | 91 | -16.624 | 5.282 | -8.790 | 1.00 | 1.17 |
| ATOM | 1335 | HN | ASN | 91 | -17.514 | 5.578 | -8.517 | 1.00 | 1.40 |
| ATOM | 1336 | CA | ASN | 91 | -15.541 | 6.286 | -9.008 | 1.00 | 1.38 |
| ATOM | 1337 | HA | ASN | 91 | -15.147 | 6.169 | -10.005 | 1.00 | 1.58 |
| ATOM | 1338 | CB | ASN | 91 | -16.116 | 7.700 | -8.857 | 1.00 | 1.87 |
| ATOM | 1339 | HB1 | ASN | 91 | -15.336 | 8.372 | -8.532 | 1.00 | 2.33 |
| ATOM | 1340 | HB2 | ASN | 91 | -16.908 | 7.686 | -8.122 | 1.00 | 1.96 |
| ATOM | 1341 | CG | ASN | 91 | -16.678 | 8.184 | -10.197 | 1.00 | 2.69 |
| ATOM | 1342 | OD1 | ASN | 91 | -16.132 | 7.890 | -11.242 | 1.00 | 3.20 |
| ATOM | 1343 | ND2 | ASN | 91 | -17.748 | 8.931 | -10.212 | 1.00 | 3.47 |
| ATOM | 1344 | HD21 | ASN | 91 | -18.186 | 9.176 | -9.370 | 1.00 | 3.59 |
| ATOM | 1345 | HD22 | ASN | 91 | -18.112 | 9.249 | -11.064 | 1.00 | 4.20 |
| ATOM | 1346 | C | ASN | 91 | -14.404 | 6.098 | -7.992 | 1.00 | 1.15 |
| ATOM | 1347 | O | ASN | 91 | -13.242 | 6.135 | -8.344 | 1.00 | 1.26 |
| ATOM | 1348 | N | TYR | 92 | -14.710 | 5.924 | -6.735 | 1.00 | 1.01 |

22/75

| | | | | | | | | | |
|------|------|-----|-----|----|---------|--------|--------|------|------|
| ATOM | 1349 | HN | TYR | 92 | -15.660 | 5.916 | -6.462 | 1.00 | 1.08 |
| ATOM | 1350 | CA | TYR | 92 | -13.639 | 5.768 | -5.711 | 1.00 | 0.97 |
| ATOM | 1351 | HA | TYR | 92 | -12.994 | 6.632 | -5.739 | 1.00 | 1.14 |
| ATOM | 1352 | CB | TYR | 92 | -14.262 | 5.652 | -4.319 | 1.00 | 1.09 |
| ATOM | 1353 | HB1 | TYR | 92 | -13.543 | 5.214 | -3.643 | 1.00 | 1.62 |
| ATOM | 1354 | HB2 | TYR | 92 | -15.135 | 5.020 | -4.369 | 1.00 | 1.45 |
| ATOM | 1355 | CG | TYR | 92 | -14.656 | 7.018 | -3.810 | 1.00 | 1.52 |
| ATOM | 1356 | CD1 | TYR | 92 | -13.672 | 7.979 | -3.549 | 1.00 | 2.14 |
| ATOM | 1357 | HD1 | TYR | 92 | -12.631 | 7.747 | -3.719 | 1.00 | 2.46 |
| ATOM | 1358 | CD2 | TYR | 92 | -16.006 | 7.320 | -3.588 | 1.00 | 2.44 |
| ATOM | 1359 | HD2 | TYR | 92 | -16.766 | 6.580 | -3.789 | 1.00 | 2.86 |
| ATOM | 1360 | CE1 | TYR | 92 | -14.037 | 9.241 | -3.066 | 1.00 | 3.06 |
| ATOM | 1361 | HE1 | TYR | 92 | -13.278 | 9.982 | -2.865 | 1.00 | 3.78 |
| ATOM | 1362 | CE2 | TYR | 92 | -16.370 | 8.582 | -3.107 | 1.00 | 3.33 |
| ATOM | 1363 | HE2 | TYR | 92 | -17.411 | 8.815 | -2.936 | 1.00 | 4.19 |
| ATOM | 1364 | CZ | TYR | 92 | -15.386 | 9.542 | -2.846 | 1.00 | 3.50 |
| ATOM | 1365 | OH | TYR | 92 | -15.746 | 10.786 | -2.368 | 1.00 | 4.57 |
| ATOM | 1366 | HH | TYR | 92 | -15.602 | 10.791 | -1.419 | 1.00 | 4.91 |
| ATOM | 1367 | C | TYR | 92 | -12.808 | 4.508 | -5.966 | 1.00 | 0.78 |
| ATOM | 1368 | O | TYR | 92 | -11.605 | 4.506 | -5.798 | 1.00 | 0.81 |
| ATOM | 1369 | N | GLY | 93 | -13.436 | 3.430 | -6.337 | 1.00 | 0.64 |
| ATOM | 1370 | HN | GLY | 93 | -14.410 | 3.441 | -6.445 | 1.00 | 0.70 |
| ATOM | 1371 | CA | GLY | 93 | -12.674 | 2.170 | -6.560 | 1.00 | 0.51 |
| ATOM | 1372 | HA1 | GLY | 93 | -13.366 | 1.366 | -6.740 | 1.00 | 0.51 |
| ATOM | 1373 | HA2 | GLY | 93 | -12.090 | 1.947 | -5.678 | 1.00 | 0.51 |
| ATOM | 1374 | C | GLY | 93 | -11.739 | 2.310 | -7.761 | 1.00 | 0.49 |
| ATOM | 1375 | O | GLY | 93 | -11.832 | 3.242 | -8.534 | 1.00 | 0.61 |
| ATOM | 1376 | N | GLY | 94 | -10.844 | 1.373 | -7.923 | 1.00 | 0.45 |
| ATOM | 1377 | HN | GLY | 94 | -10.799 | 0.627 | -7.288 | 1.00 | 0.44 |
| ATOM | 1378 | CA | GLY | 94 | -9.902 | 1.420 | -9.075 | 1.00 | 0.55 |
| ATOM | 1379 | HA1 | GLY | 94 | -10.459 | 1.569 | -9.988 | 1.00 | 0.63 |
| ATOM | 1380 | HA2 | GLY | 94 | -9.363 | 0.485 | -9.133 | 1.00 | 0.58 |
| ATOM | 1381 | C | GLY | 94 | -8.905 | 2.569 | -8.901 | 1.00 | 0.60 |
| ATOM | 1382 | O | GLY | 94 | -8.109 | 2.838 | -9.772 | 1.00 | 1.14 |
| ATOM | 1383 | N | ASP | 95 | -8.933 | 3.252 | -7.790 | 1.00 | 0.24 |
| ATOM | 1384 | HN | ASP | 95 | -9.581 | 3.028 | -7.089 | 1.00 | 0.52 |
| ATOM | 1385 | CA | ASP | 95 | -7.976 | 4.382 | -7.597 | 1.00 | 0.24 |
| ATOM | 1386 | HA | ASP | 95 | -7.888 | 4.939 | -8.518 | 1.00 | 0.28 |
| ATOM | 1387 | CB | ASP | 95 | -8.493 | 5.303 | -6.491 | 1.00 | 0.26 |
| ATOM | 1388 | HB1 | ASP | 95 | -9.500 | 5.617 | -6.724 | 1.00 | 0.28 |
| ATOM | 1389 | HB2 | ASP | 95 | -7.853 | 6.170 | -6.415 | 1.00 | 0.30 |
| ATOM | 1390 | CG | ASP | 95 | -8.494 | 4.549 | -5.162 | 1.00 | 0.28 |
| ATOM | 1391 | OD1 | ASP | 95 | -8.543 | 5.200 | -4.132 | 1.00 | 1.08 |
| ATOM | 1392 | OD2 | ASP | 95 | -8.440 | 3.331 | -5.198 | 1.00 | 1.14 |
| ATOM | 1393 | C | ASP | 95 | -6.605 | 3.827 | -7.202 | 1.00 | 0.23 |
| ATOM | 1394 | O | ASP | 95 | -6.479 | 2.683 | -6.815 | 1.00 | 0.24 |
| ATOM | 1395 | N | ALA | 96 | -5.573 | 4.626 | -7.297 | 1.00 | 0.23 |
| ATOM | 1396 | HN | ALA | 96 | -5.692 | 5.546 | -7.614 | 1.00 | 0.23 |
| ATOM | 1397 | CA | ALA | 96 | -4.215 | 4.131 | -6.926 | 1.00 | 0.25 |
| ATOM | 1398 | HA | ALA | 96 | -4.307 | 3.360 | -6.175 | 1.00 | 0.25 |
| ATOM | 1399 | CB | ALA | 96 | -3.527 | 3.553 | -8.164 | 1.00 | 0.30 |
| ATOM | 1400 | HB1 | ALA | 96 | -2.528 | 3.236 | -7.905 | 1.00 | 1.08 |
| ATOM | 1401 | HB2 | ALA | 96 | -3.476 | 4.309 | -8.934 | 1.00 | 1.08 |
| ATOM | 1402 | HB3 | ALA | 96 | -4.090 | 2.706 | -8.528 | 1.00 | 1.03 |
| ATOM | 1403 | C | ALA | 96 | -3.375 | 5.284 | -6.372 | 1.00 | 0.25 |
| ATOM | 1404 | O | ALA | 96 | -3.222 | 6.313 | -7.005 | 1.00 | 0.29 |
| ATOM | 1405 | N | HXS | 97 | -2.831 | 5.113 | -5.192 | 1.00 | 0.25 |
| ATOM | 1406 | HN | HXS | 97 | -2.976 | 4.271 | -4.710 | 1.00 | 0.28 |
| ATOM | 1407 | CA | HXS | 97 | -1.996 | 6.187 | -4.574 | 1.00 | 0.27 |
| ATOM | 1408 | HA | HXS | 97 | -2.010 | 7.068 | -5.198 | 1.00 | 0.28 |
| ATOM | 1409 | CB | HXS | 97 | -2.564 | 6.537 | -3.197 | 1.00 | 0.33 |
| ATOM | 1410 | HB1 | HXS | 97 | -1.969 | 7.319 | -2.750 | 1.00 | 0.44 |
| ATOM | 1411 | HB2 | HXS | 97 | -2.540 | 5.661 | -2.566 | 1.00 | 0.39 |
| ATOM | 1412 | CG | HXS | 97 | -3.983 | 7.009 | -3.349 | 1.00 | 0.37 |
| ATOM | 1413 | ND1 | HXS | 97 | -4.697 | 7.052 | -2.163 | 1.00 | 0.80 |
| ATOM | 1414 | CD2 | HXS | 97 | -4.783 | 7.420 | -4.384 | 1.00 | 0.55 |
| ATOM | 1415 | HD2 | HXS | 97 | -4.517 | 7.497 | -5.428 | 1.00 | 0.94 |
| ATOM | 1416 | CE1 | HXS | 97 | -5.918 | 7.487 | -2.498 | 1.00 | 0.86 |
| ATOM | 1417 | HE1 | HXS | 97 | -6.724 | 7.632 | -1.795 | 1.00 | 1.24 |
| ATOM | 1418 | NE2 | HXS | 97 | -6.018 | 7.722 | -3.819 | 1.00 | 0.59 |
| ATOM | 1419 | HE2 | HXS | 97 | -6.812 | 8.044 | -4.294 | 1.00 | 0.72 |
| ATOM | 1420 | C | HXS | 97 | -0.552 | 5.700 | -4.420 | 1.00 | 0.26 |
| ATOM | 1421 | O | HXS | 97 | -0.299 | 4.525 | -4.237 | 1.00 | 0.39 |
| ATOM | 1422 | N | PHE | 98 | 0.391 | 6.604 | -4.496 | 1.00 | 0.18 |
| ATOM | 1423 | HN | PHE | 98 | 0.147 | 7.540 | -4.648 | 1.00 | 0.23 |
| ATOM | 1424 | CA | PHE | 98 | 1.832 | 6.230 | -4.360 | 1.00 | 0.17 |
| ATOM | 1425 | HA | PHE | 98 | 1.921 | 5.190 | -4.085 | 1.00 | 0.18 |

23/75

| | | | | | | | | | |
|------|------|------|-----|-----|--------|--------|--------|------|------|
| ATOM | 1426 | CB | PHE | 98 | 2.543 | 6.472 | -5.691 | 1.00 | 0.18 |
| ATOM | 1427 | HB1 | PHE | 98 | 3.611 | 6.464 | -5.536 | 1.00 | 0.21 |
| ATOM | 1428 | HB2 | PHE | 98 | 2.243 | 7.431 | -6.085 | 1.00 | 0.20 |
| ATOM | 1429 | CG | PHE | 98 | 2.169 | 5.391 | -6.674 | 1.00 | 0.19 |
| ATOM | 1430 | CD1 | PHE | 98 | 3.114 | 4.428 | -7.048 | 1.00 | 0.22 |
| ATOM | 1431 | HD1 | PHE | 98 | 4.110 | 4.456 | -6.631 | 1.00 | 0.25 |
| ATOM | 1432 | CD2 | PHE | 98 | 0.880 | 5.355 | -7.214 | 1.00 | 0.22 |
| ATOM | 1433 | HD2 | PHE | 98 | 0.151 | 6.098 | -6.924 | 1.00 | 0.24 |
| ATOM | 1434 | CE1 | PHE | 98 | 2.768 | 3.429 | -7.963 | 1.00 | 0.25 |
| ATOM | 1435 | HE1 | PHE | 98 | 3.496 | 2.685 | -8.252 | 1.00 | 0.29 |
| ATOM | 1436 | CE2 | PHE | 98 | 0.533 | 4.355 | -8.127 | 1.00 | 0.26 |
| ATOM | 1437 | HE2 | PHE | 98 | -0.462 | 4.327 | -8.542 | 1.00 | 0.31 |
| ATOM | 1438 | CZ | PHE | 98 | 1.478 | 3.392 | -8.503 | 1.00 | 0.26 |
| ATOM | 1439 | HZ | PHE | 98 | 1.214 | 2.622 | -9.211 | 1.00 | 0.30 |
| ATOM | 1440 | C | PHE | 98 | 2.487 | 7.104 | -3.286 | 1.00 | 0.17 |
| ATOM | 1441 | O | PHE | 98 | 2.081 | 8.226 | -3.058 | 1.00 | 0.19 |
| ATOM | 1442 | N | ASP | 99 | 3.498 | 6.604 | -2.625 | 1.00 | 0.19 |
| ATOM | 1443 | HN | ASP | 99 | 3.813 | 5.693 | -2.820 | 1.00 | 0.22 |
| ATOM | 1444 | CA | ASP | 99 | 4.167 | 7.424 | -1.570 | 1.00 | 0.20 |
| ATOM | 1445 | HA | ASP | 99 | 3.421 | 7.956 | -0.998 | 1.00 | 0.20 |
| ATOM | 1446 | CB | ASP | 99 | 4.973 | 6.516 | -0.638 | 1.00 | 0.25 |
| ATOM | 1447 | HB1 | ASP | 99 | 5.567 | 7.122 | 0.029 | 1.00 | 0.28 |
| ATOM | 1448 | HB2 | ASP | 99 | 5.624 | 5.884 | -1.226 | 1.00 | 0.30 |
| ATOM | 1449 | CG | ASP | 99 | 4.023 | 5.646 | 0.180 | 1.00 | 0.41 |
| ATOM | 1450 | OD1 | ASP | 99 | 2.838 | 5.680 | -0.100 | 1.00 | 0.89 |
| ATOM | 1451 | OD2 | ASP | 99 | 4.497 | 4.968 | 1.079 | 1.00 | 0.27 |
| ATOM | 1452 | C | ASP | 99 | 5.123 | 8.426 | -2.224 | 1.00 | 0.21 |
| ATOM | 1453 | O | ASP | 99 | 6.020 | 8.054 | -2.954 | 1.00 | 0.25 |
| ATOM | 1454 | N | ASP | 100 | 4.946 | 9.694 | -1.962 | 1.00 | 0.23 |
| ATOM | 1455 | HN | ASP | 100 | 4.222 | 9.976 | -1.365 | 1.00 | 0.23 |
| ATOM | 1456 | CA | ASP | 100 | 5.857 | 10.710 | -2.565 | 1.00 | 0.29 |
| ATOM | 1457 | HA | ASP | 100 | 6.169 | 10.379 | -3.545 | 1.00 | 0.31 |
| ATOM | 1458 | CB | ASP | 100 | 5.127 | 12.049 | -2.684 | 1.00 | 0.34 |
| ATOM | 1459 | HB1 | ASP | 100 | 5.130 | 12.544 | -1.727 | 1.00 | 0.34 |
| ATOM | 1460 | HB2 | ASP | 100 | 4.109 | 11.879 | -2.999 | 1.00 | 0.34 |
| ATOM | 1461 | CG | ASP | 100 | 5.844 | 12.929 | -3.710 | 1.00 | 0.43 |
| ATOM | 1462 | OD1 | ASP | 100 | 5.240 | 13.887 | -4.164 | 1.00 | 1.21 |
| ATOM | 1463 | OD2 | ASP | 100 | 6.984 | 12.630 | -4.025 | 1.00 | 1.12 |
| ATOM | 1464 | C | ASP | 100 | 7.085 | 10.885 | -1.667 | 1.00 | 0.30 |
| ATOM | 1465 | O | ASP | 100 | 8.032 | 11.559 | -2.018 | 1.00 | 0.32 |
| ATOM | 1466 | N | ASP | 101 | 7.074 | 10.280 | -0.510 | 1.00 | 0.31 |
| ATOM | 1467 | HN | ASP | 101 | 6.298 | 9.741 | -0.249 | 1.00 | 0.32 |
| ATOM | 1468 | CA | ASP | 101 | 8.236 | 10.407 | 0.415 | 1.00 | 0.33 |
| ATOM | 1469 | HA | ASP | 101 | 8.647 | 11.403 | 0.345 | 1.00 | 0.36 |
| ATOM | 1470 | CB | ASP | 101 | 7.778 | 10.142 | 1.851 | 1.00 | 0.39 |
| ATOM | 1471 | HB1 | ASP | 101 | 8.641 | 10.060 | 2.495 | 1.00 | 0.41 |
| ATOM | 1472 | HB2 | ASP | 101 | 7.216 | 9.220 | 1.884 | 1.00 | 0.39 |
| ATOM | 1473 | CG | ASP | 101 | 6.896 | 11.296 | 2.330 | 1.00 | 0.45 |
| ATOM | 1474 | OD1 | ASP | 101 | 7.027 | 12.380 | 1.786 | 1.00 | 1.25 |
| ATOM | 1475 | OD2 | ASP | 101 | 6.104 | 11.076 | 3.231 | 1.00 | 1.09 |
| ATOM | 1476 | C | ASP | 101 | 9.304 | 9.385 | 0.028 | 1.00 | 0.30 |
| ATOM | 1477 | O | ASP | 101 | 10.411 | 9.405 | 0.529 | 1.00 | 0.29 |
| ATOM | 1478 | N | GLU | 102 | 8.971 | 8.484 | -0.849 | 1.00 | 0.30 |
| ATOM | 1479 | HN | GLU | 102 | 8.068 | 8.484 | -1.230 | 1.00 | 0.31 |
| ATOM | 1480 | CA | GLU | 102 | 9.950 | 7.444 | -1.266 | 1.00 | 0.29 |
| ATOM | 1481 | HA | GLU | 102 | 10.649 | 7.263 | -0.463 | 1.00 | 0.30 |
| ATOM | 1482 | CB | GLU | 102 | 9.195 | 6.155 | -1.585 | 1.00 | 0.35 |
| ATOM | 1483 | HB1 | GLU | 102 | 9.873 | 5.437 | -2.020 | 1.00 | 0.36 |
| ATOM | 1484 | HB2 | GLU | 102 | 8.397 | 6.368 | -2.282 | 1.00 | 0.40 |
| ATOM | 1485 | CG | GLU | 102 | 8.611 | 5.584 | -0.293 | 1.00 | 0.46 |
| ATOM | 1486 | HG1 | GLU | 102 | 8.020 | 6.342 | 0.200 | 1.00 | 1.18 |
| ATOM | 1487 | HG2 | GLU | 102 | 9.415 | 5.276 | 0.356 | 1.00 | 1.03 |
| ATOM | 1488 | CD | GLU | 102 | 7.724 | 4.381 | -0.616 | 1.00 | 0.83 |
| ATOM | 1489 | OE1 | GLU | 102 | 7.601 | 4.060 | -1.786 | 1.00 | 1.63 |
| ATOM | 1490 | OE2 | GLU | 102 | 7.184 | 3.801 | 0.314 | 1.00 | 0.87 |
| ATOM | 1491 | C | GLU | 102 | 10.707 | 7.917 | -2.508 | 1.00 | 0.25 |
| ATOM | 1492 | O | GLU | 102 | 10.359 | 8.910 | -3.115 | 1.00 | 0.25 |
| ATOM | 1493 | N | THR | 103 | 11.741 | 7.213 | -2.886 | 1.00 | 0.25 |
| ATOM | 1494 | HN | THR | 103 | 12.003 | 6.416 | -2.379 | 1.00 | 0.28 |
| ATOM | 1495 | CA | THR | 103 | 12.525 | 7.620 | -4.088 | 1.00 | 0.23 |
| ATOM | 1496 | HA | THR | 103 | 12.356 | 8.665 | -4.301 | 1.00 | 0.23 |
| ATOM | 1497 | CB | THR | 103 | 14.016 | 7.383 | -3.824 | 1.00 | 0.27 |
| ATOM | 1498 | HB | THR | 103 | 14.169 | 6.359 | -3.521 | 1.00 | 0.30 |
| ATOM | 1499 | OG1 | THR | 103 | 14.455 | 8.252 | -2.789 | 1.00 | 0.29 |
| ATOM | 1500 | HG1 | THR | 103 | 15.334 | 8.564 | -3.016 | 1.00 | 0.86 |
| ATOM | 1501 | CG2 | THR | 103 | 14.820 | 7.656 | -5.098 | 1.00 | 0.29 |
| ATOM | 1502 | HG21 | THR | 103 | 15.864 | 7.777 | -4.846 | 1.00 | 1.00 |

24/75

| | | | | | | | | | |
|------|------|------|-----|-----|--------|--------|---------|------|------|
| ATOM | 1503 | HG22 | THR | 103 | 14.457 | 8.557 | -5.569 | 1.00 | 1.08 |
| ATOM | 1504 | HG23 | THR | 103 | 14.710 | 6.824 | -5.779 | 1.00 | 1.01 |
| ATOM | 1505 | C | THR | 103 | 12.083 | 6.777 | -5.281 | 1.00 | 0.22 |
| ATOM | 1506 | O | THR | 103 | 12.417 | 5.614 | -5.394 | 1.00 | 0.23 |
| ATOM | 1507 | N | TRP | 104 | 11.332 | 7.358 | -6.175 | 1.00 | 0.21 |
| ATOM | 1508 | HN | TRP | 104 | 11.076 | 8.297 | -6.063 | 1.00 | 0.23 |
| ATOM | 1509 | CA | TRP | 104 | 10.867 | 6.598 | -7.364 | 1.00 | 0.21 |
| ATOM | 1510 | HA | TRP | 104 | 10.750 | 5.556 | -7.104 | 1.00 | 0.20 |
| ATOM | 1511 | CB | TRP | 104 | 9.525 | 7.165 | -7.831 | 1.00 | 0.23 |
| ATOM | 1512 | HB1 | TRP | 104 | 9.188 | 6.623 | -8.702 | 1.00 | 0.24 |
| ATOM | 1513 | HB2 | TRP | 104 | 9.641 | 8.210 | -8.078 | 1.00 | 0.25 |
| ATOM | 1514 | CG | TRP | 104 | 8.520 | 7.018 | -6.731 | 1.00 | 0.24 |
| ATOM | 1515 | CD1 | TRP | 104 | 8.098 | 8.019 | -5.924 | 1.00 | 0.31 |
| ATOM | 1516 | HD1 | TRP | 104 | 8.427 | 9.045 | -5.972 | 1.00 | 0.36 |
| ATOM | 1517 | CD2 | TRP | 104 | 7.811 | 5.821 | -6.300 | 1.00 | 0.21 |
| ATOM | 1518 | NE1 | TRP | 104 | 7.176 | 7.512 | -5.026 | 1.00 | 0.31 |
| ATOM | 1519 | HE1 | TRP | 104 | 6.718 | 8.030 | -4.331 | 1.00 | 0.36 |
| ATOM | 1520 | CE2 | TRP | 104 | 6.963 | 6.162 | -5.220 | 1.00 | 0.24 |
| ATOM | 1521 | CE3 | TRP | 104 | 7.819 | 4.486 | -6.739 | 1.00 | 0.18 |
| ATOM | 1522 | HE3 | TRP | 104 | 8.458 | 4.198 | -7.559 | 1.00 | 0.19 |
| ATOM | 1523 | CZ2 | TRP | 104 | 6.153 | 5.213 | -4.596 | 1.00 | 0.23 |
| ATOM | 1524 | HZ2 | TRP | 104 | 5.515 | 5.499 | -3.774 | 1.00 | 0.27 |
| ATOM | 1525 | CZ3 | TRP | 104 | 7.005 | 3.527 | -6.114 | 1.00 | 0.20 |
| ATOM | 1526 | HZ3 | TRP | 104 | 7.019 | 2.504 | -6.460 | 1.00 | 0.23 |
| ATOM | 1527 | CH2 | TRP | 104 | 6.173 | 3.891 | -5.045 | 1.00 | 0.21 |
| ATOM | 1528 | HH2 | TRP | 104 | 5.548 | 3.150 | -4.568 | 1.00 | 0.23 |
| ATOM | 1529 | C | TRP | 104 | 11.911 | 6.732 | -8.474 | 1.00 | 0.21 |
| ATOM | 1530 | O | TRP | 104 | 12.276 | 7.824 | -8.864 | 1.00 | 0.24 |
| ATOM | 1531 | N | THR | 105 | 12.403 | 5.630 | -8.973 | 1.00 | 0.20 |
| ATOM | 1532 | HN | THR | 105 | 12.098 | 4.763 | -8.633 | 1.00 | 0.19 |
| ATOM | 1533 | CA | THR | 105 | 13.437 | 5.685 | -10.048 | 1.00 | 0.21 |
| ATOM | 1534 | HA | THR | 105 | 13.415 | 6.652 | -10.525 | 1.00 | 0.24 |
| ATOM | 1535 | CB | THR | 105 | 14.817 | 5.459 | -9.428 | 1.00 | 0.21 |
| ATOM | 1536 | HB | THR | 105 | 15.018 | 6.233 | -8.704 | 1.00 | 0.21 |
| ATOM | 1537 | OG1 | THR | 105 | 15.806 | 5.497 | -10.447 | 1.00 | 0.24 |
| ATOM | 1538 | HG1 | THR | 105 | 15.882 | 6.404 | -10.752 | 1.00 | 0.86 |
| ATOM | 1539 | CG2 | THR | 105 | 14.846 | 4.101 | -8.729 | 1.00 | 0.21 |
| ATOM | 1540 | HG21 | THR | 105 | 15.178 | 4.233 | -7.711 | 1.00 | 1.04 |
| ATOM | 1541 | HG22 | THR | 105 | 15.524 | 3.442 | -9.249 | 1.00 | 1.07 |
| ATOM | 1542 | HG23 | THR | 105 | 13.854 | 3.674 | -8.731 | 1.00 | 0.99 |
| ATOM | 1543 | C | THR | 105 | 13.166 | 4.597 | -11.087 | 1.00 | 0.23 |
| ATOM | 1544 | O | THR | 105 | 12.521 | 3.606 | -10.808 | 1.00 | 0.23 |
| ATOM | 1545 | N | SER | 106 | 13.668 | 4.769 | -12.282 | 1.00 | 0.26 |
| ATOM | 1546 | HN | SER | 106 | 14.194 | 5.572 | -12.480 | 1.00 | 0.29 |
| ATOM | 1547 | CA | SER | 106 | 13.454 | 3.739 | -13.337 | 1.00 | 0.29 |
| ATOM | 1548 | HA | SER | 106 | 12.570 | 3.163 | -13.111 | 1.00 | 0.30 |
| ATOM | 1549 | CB | SER | 106 | 13.290 | 4.423 | -14.695 | 1.00 | 0.35 |
| ATOM | 1550 | HB1 | SER | 106 | 14.249 | 4.467 | -15.193 | 1.00 | 1.09 |
| ATOM | 1551 | HB2 | SER | 106 | 12.916 | 5.424 | -14.554 | 1.00 | 0.96 |
| ATOM | 1552 | OG | SER | 106 | 12.365 | 3.685 | -15.483 | 1.00 | 1.44 |
| ATOM | 1553 | HG | SER | 106 | 11.671 | 4.285 | -15.766 | 1.00 | 1.97 |
| ATOM | 1554 | C | SER | 106 | 14.674 | 2.817 | -13.372 | 1.00 | 0.28 |
| ATOM | 1555 | O | SER | 106 | 14.669 | 1.781 | -14.006 | 1.00 | 0.31 |
| ATOM | 1556 | N | SER | 107 | 15.715 | 3.187 | -12.677 | 1.00 | 0.26 |
| ATOM | 1557 | HN | SER | 107 | 15.687 | 4.023 | -12.166 | 1.00 | 0.25 |
| ATOM | 1558 | CA | SER | 107 | 16.940 | 2.340 | -12.641 | 1.00 | 0.27 |
| ATOM | 1559 | HA | SER | 107 | 17.018 | 1.778 | -13.560 | 1.00 | 0.29 |
| ATOM | 1560 | CB | SER | 107 | 18.175 | 3.226 | -12.474 | 1.00 | 0.28 |
| ATOM | 1561 | HB1 | SER | 107 | 18.292 | 3.847 | -13.353 | 1.00 | 1.12 |
| ATOM | 1562 | HB2 | SER | 107 | 19.049 | 2.609 | -12.355 | 1.00 | 1.04 |
| ATOM | 1563 | OG | SER | 107 | 18.017 | 4.040 | -11.320 | 1.00 | 1.29 |
| ATOM | 1564 | HG | SER | 107 | 18.556 | 4.827 | -11.436 | 1.00 | 1.82 |
| ATOM | 1565 | C | SER | 107 | 16.836 | 1.376 | -11.460 | 1.00 | 0.26 |
| ATOM | 1566 | O | SER | 107 | 15.829 | 1.324 | -10.781 | 1.00 | 0.26 |
| ATOM | 1567 | N | SER | 108 | 17.859 | 0.609 | -11.203 | 1.00 | 0.28 |
| ATOM | 1568 | HN | SER | 108 | 18.666 | 0.658 | -11.757 | 1.00 | 0.31 |
| ATOM | 1569 | CA | SER | 108 | 17.788 | -0.342 | -10.061 | 1.00 | 0.30 |
| ATOM | 1570 | HA | SER | 108 | 16.775 | -0.706 | -9.967 | 1.00 | 0.30 |
| ATOM | 1571 | CB | SER | 108 | 18.728 | -1.527 | -10.330 | 1.00 | 0.36 |
| ATOM | 1572 | HB1 | SER | 108 | 19.561 | -1.505 | -9.642 | 1.00 | 1.09 |
| ATOM | 1573 | HB2 | SER | 108 | 19.103 | -1.468 | -11.338 | 1.00 | 0.95 |
| ATOM | 1574 | OG | SER | 108 | 18.005 | -2.741 | -10.176 | 1.00 | 1.47 |
| ATOM | 1575 | HG | SER | 108 | 18.550 | -3.456 | -10.513 | 1.00 | 2.00 |
| ATOM | 1576 | C | SER | 108 | 18.181 | 0.390 | -8.767 | 1.00 | 0.28 |
| ATOM | 1577 | O | SER | 108 | 19.279 | 0.265 | -8.261 | 1.00 | 0.33 |
| ATOM | 1578 | N | LYS | 109 | 17.272 | 1.157 | -8.224 | 1.00 | 0.24 |
| ATOM | 1579 | HN | LYS | 109 | 16.362 | 1.241 | -8.646 | 1.00 | 0.22 |

25/75

| | | | | | | | | | |
|------|------|------|-----|-----|--------|--------|---------|------|------|
| ATOM | 1580 | CA | LYS | 109 | 17.561 | 1.897 | -6.960 | 1.00 | 0.23 |
| ATOM | 1581 | HA | LYS | 109 | 18.275 | 1.341 | -6.370 | 1.00 | 0.25 |
| ATOM | 1582 | CB | LYS | 109 | 18.123 | 3.293 | -7.268 | 1.00 | 0.24 |
| ATOM | 1583 | HB1 | LYS | 109 | 18.172 | 3.868 | -6.355 | 1.00 | 0.27 |
| ATOM | 1584 | HB2 | LYS | 109 | 17.472 | 3.793 | -7.970 | 1.00 | 0.25 |
| ATOM | 1585 | CG | LYS | 109 | 19.525 | 3.177 | -7.868 | 1.00 | 0.30 |
| ATOM | 1586 | HG1 | LYS | 109 | 19.476 | 2.615 | -8.785 | 1.00 | 0.54 |
| ATOM | 1587 | HG2 | LYS | 109 | 20.177 | 2.675 | -7.170 | 1.00 | 0.70 |
| ATOM | 1588 | CD | LYS | 109 | 20.072 | 4.574 | -8.169 | 1.00 | 0.75 |
| ATOM | 1589 | HD1 | LYS | 109 | 20.124 | 5.144 | -7.254 | 1.00 | 1.27 |
| ATOM | 1590 | HD2 | LYS | 109 | 19.420 | 5.074 | -8.870 | 1.00 | 1.27 |
| ATOM | 1591 | CE | LYS | 109 | 21.475 | 4.453 | -8.770 | 1.00 | 1.13 |
| ATOM | 1592 | HE1 | LYS | 109 | 21.396 | 4.264 | -9.830 | 1.00 | 1.68 |
| ATOM | 1593 | HE2 | LYS | 109 | 22.000 | 3.636 | -8.297 | 1.00 | 1.68 |
| ATOM | 1594 | NZ | LYS | 109 | 22.224 | 5.721 | -8.545 | 1.00 | 1.79 |
| ATOM | 1595 | HZ1 | LYS | 109 | 21.689 | 6.516 | -8.948 | 1.00 | 2.22 |
| ATOM | 1596 | HZ2 | LYS | 109 | 23.155 | 5.660 | -9.006 | 1.00 | 2.17 |
| ATOM | 1597 | HZ3 | LYS | 109 | 22.351 | 5.873 | -7.525 | 1.00 | 2.34 |
| ATOM | 1598 | C | LYS | 109 | 16.259 | 2.052 | -6.175 | 1.00 | 0.21 |
| ATOM | 1599 | O | LYS | 109 | 15.190 | 2.110 | -6.747 | 1.00 | 0.20 |
| ATOM | 1600 | N | GLY | 110 | 16.338 | 2.124 | -4.873 | 1.00 | 0.23 |
| ATOM | 1601 | HN | GLY | 110 | 17.212 | 2.079 | -4.432 | 1.00 | 0.26 |
| ATOM | 1602 | CA | GLY | 110 | 15.099 | 2.283 | -4.056 | 1.00 | 0.22 |
| ATOM | 1603 | HA1 | GLY | 110 | 14.751 | 3.302 | -4.124 | 1.00 | 0.23 |
| ATOM | 1604 | HA2 | GLY | 110 | 15.316 | 2.044 | -3.024 | 1.00 | 0.25 |
| ATOM | 1605 | C | GLY | 110 | 14.013 | 1.342 | -4.581 | 1.00 | 0.19 |
| ATOM | 1606 | O | GLY | 110 | 14.281 | 0.216 | -4.949 | 1.00 | 0.20 |
| ATOM | 1607 | N | TYR | 111 | 12.789 | 1.801 | -4.626 | 1.00 | 0.17 |
| ATOM | 1608 | HN | TYR | 111 | 12.599 | 2.716 | -4.330 | 1.00 | 0.18 |
| ATOM | 1609 | CA | TYR | 111 | 11.683 | 0.941 | -5.136 | 1.00 | 0.15 |
| ATOM | 1610 | HA | TYR | 111 | 11.975 | -0.098 | -5.088 | 1.00 | 0.16 |
| ATOM | 1611 | CB | TYR | 111 | 10.437 | 1.162 | -4.277 | 1.00 | 0.15 |
| ATOM | 1612 | HB1 | TYR | 111 | 9.633 | 0.540 | -4.641 | 1.00 | 0.15 |
| ATOM | 1613 | HB2 | TYR | 111 | 10.143 | 2.200 | -4.330 | 1.00 | 0.16 |
| ATOM | 1614 | CG | TYR | 111 | 10.745 | 0.798 | -2.844 | 1.00 | 0.17 |
| ATOM | 1615 | CD1 | TYR | 111 | 10.648 | -0.533 | -2.422 | 1.00 | 0.17 |
| ATOM | 1616 | HD1 | TYR | 111 | 10.354 | -1.301 | -3.121 | 1.00 | 0.17 |
| ATOM | 1617 | CD2 | TYR | 111 | 11.127 | 1.794 | -1.936 | 1.00 | 0.20 |
| ATOM | 1618 | HD2 | TYR | 111 | 11.201 | 2.821 | -2.261 | 1.00 | 0.23 |
| ATOM | 1619 | CE1 | TYR | 111 | 10.933 | -0.868 | -1.093 | 1.00 | 0.19 |
| ATOM | 1620 | HE1 | TYR | 111 | 10.858 | -1.895 | -0.767 | 1.00 | 0.20 |
| ATOM | 1621 | CE2 | TYR | 111 | 11.412 | 1.459 | -0.607 | 1.00 | 0.22 |
| ATOM | 1622 | HE2 | TYR | 111 | 11.706 | 2.227 | 0.093 | 1.00 | 0.26 |
| ATOM | 1623 | CZ | TYR | 111 | 11.315 | 0.127 | -0.185 | 1.00 | 0.21 |
| ATOM | 1624 | OH | TYR | 111 | 11.595 | -0.204 | 1.125 | 1.00 | 0.23 |
| ATOM | 1625 | HH | TYR | 111 | 12.543 | -0.121 | 1.255 | 1.00 | 0.95 |
| ATOM | 1626 | C | TYR | 111 | 11.374 | 1.321 | -6.588 | 1.00 | 0.14 |
| ATOM | 1627 | O | TYR | 111 | 10.949 | 2.424 | -6.871 | 1.00 | 0.15 |
| ATOM | 1628 | N | ASN | 112 | 11.581 | 0.421 | -7.511 | 1.00 | 0.15 |
| ATOM | 1629 | HN | ASN | 112 | 11.924 | -0.464 | -7.264 | 1.00 | 0.17 |
| ATOM | 1630 | CA | ASN | 112 | 11.295 | 0.739 | -8.939 | 1.00 | 0.16 |
| ATOM | 1631 | HA | ASN | 112 | 11.870 | 1.605 | -9.235 | 1.00 | 0.16 |
| ATOM | 1632 | CB | ASN | 112 | 11.677 | -0.450 | -9.822 | 1.00 | 0.19 |
| ATOM | 1633 | HB1 | ASN | 112 | 11.025 | -1.276 | -9.607 | 1.00 | 0.22 |
| ATOM | 1634 | HB2 | ASN | 112 | 12.698 | -0.739 | -9.622 | 1.00 | 0.19 |
| ATOM | 1635 | CG | ASN | 112 | 11.531 | -0.060 | -11.295 | 1.00 | 0.24 |
| ATOM | 1636 | OD1 | ASN | 112 | 10.446 | 0.248 | -11.748 | 1.00 | 0.96 |
| ATOM | 1637 | ND2 | ASN | 112 | 12.583 | -0.059 | -12.067 | 1.00 | 1.06 |
| ATOM | 1638 | HD21 | ASN | 112 | 13.458 | -0.308 | -11.704 | 1.00 | 1.80 |
| ATOM | 1639 | HD22 | ASN | 112 | 12.497 | 0.189 | -13.012 | 1.00 | 1.08 |
| ATOM | 1640 | C | ASN | 112 | 9.803 | 1.040 | -9.108 | 1.00 | 0.15 |
| ATOM | 1641 | O | ASN | 112 | 8.953 | 0.310 | -8.637 | 1.00 | 0.14 |
| ATOM | 1642 | N | LEU | 113 | 9.482 | 2.112 | -9.777 | 1.00 | 0.15 |
| ATOM | 1643 | HN | LEU | 113 | 10.187 | 2.684 | -10.145 | 1.00 | 0.16 |
| ATOM | 1644 | CA | LEU | 113 | 8.049 | 2.475 | -9.984 | 1.00 | 0.15 |
| ATOM | 1645 | HA | LEU | 113 | 7.582 | 2.620 | -9.025 | 1.00 | 0.14 |
| ATOM | 1646 | CB | LEU | 113 | 7.981 | 3.781 | -10.791 | 1.00 | 0.16 |
| ATOM | 1647 | HB1 | LEU | 113 | 8.513 | 3.646 | -11.721 | 1.00 | 0.17 |
| ATOM | 1648 | HB2 | LEU | 113 | 8.452 | 4.571 | -10.226 | 1.00 | 0.16 |
| ATOM | 1649 | CG | LEU | 113 | 6.523 | 4.177 | -11.095 | 1.00 | 0.17 |
| ATOM | 1650 | HG | LEU | 113 | 6.041 | 3.387 | -11.652 | 1.00 | 0.18 |
| ATOM | 1651 | CD1 | LEU | 113 | 5.748 | 4.421 | -9.793 | 1.00 | 0.18 |
| ATOM | 1652 | HD11 | LEU | 113 | 4.841 | 4.969 | -10.007 | 1.00 | 0.99 |
| ATOM | 1653 | HD12 | LEU | 113 | 6.359 | 4.991 | -9.110 | 1.00 | 1.00 |
| ATOM | 1654 | HD13 | LEU | 113 | 5.490 | 3.474 | -9.343 | 1.00 | 0.97 |
| ATOM | 1655 | CD2 | LEU | 113 | 6.526 | 5.457 | -11.943 | 1.00 | 0.20 |
| ATOM | 1656 | HD21 | LEU | 113 | 6.116 | 6.377 | -11.374 | 1.00 | 1.26 |

26/75

| | | | | | | | | | |
|------|------|------|-----|-----|--------|--------|---------|------|------|
| ATOM | 1657 | HD22 | LEU | 113 | 5.930 | 5.302 | -12.830 | 1.00 | 1.03 |
| ATOM | 1658 | HD23 | LEU | 113 | 7.539 | 5.696 | -12.231 | 1.00 | 1.00 |
| ATOM | 1659 | C | LEU | 113 | 7.320 | 1.361 | -10.743 | 1.00 | 0.15 |
| ATOM | 1660 | O | LEU | 113 | 6.203 | 1.014 | -10.419 | 1.00 | 0.15 |
| ATOM | 1661 | N | PHE | 114 | 7.928 | 0.817 | -11.762 | 1.00 | 0.16 |
| ATOM | 1662 | HN | PHE | 114 | 8.822 | 1.123 | -12.020 | 1.00 | 0.17 |
| ATOM | 1663 | CA | PHE | 114 | 7.245 | -0.250 | -12.555 | 1.00 | 0.17 |
| ATOM | 1664 | HA | PHE | 114 | 6.338 | 0.151 | -12.980 | 1.00 | 0.18 |
| ATOM | 1665 | CB | PHE | 114 | 8.159 | -0.720 | -13.685 | 1.00 | 0.21 |
| ATOM | 1666 | HB1 | PHE | 114 | 9.077 | -1.108 | -13.271 | 1.00 | 0.22 |
| ATOM | 1667 | HB2 | PHE | 114 | 8.380 | 0.111 | -14.340 | 1.00 | 0.22 |
| ATOM | 1668 | CG | PHE | 114 | 7.457 | -1.807 | -14.464 | 1.00 | 0.24 |
| ATOM | 1669 | CD1 | PHE | 114 | 7.545 | -3.135 | -14.031 | 1.00 | 0.35 |
| ATOM | 1670 | HD1 | PHE | 114 | 8.105 | -3.376 | -13.147 | 1.00 | 0.43 |
| ATOM | 1671 | CD2 | PHE | 114 | 6.724 | -1.494 | -15.613 | 1.00 | 0.24 |
| ATOM | 1672 | HD2 | PHE | 114 | 6.655 | -0.470 | -15.950 | 1.00 | 0.28 |
| ATOM | 1673 | CE1 | PHE | 114 | 6.902 | -4.149 | -14.741 | 1.00 | 0.39 |
| ATOM | 1674 | HE1 | PHE | 114 | 6.975 | -5.171 | -14.402 | 1.00 | 0.50 |
| ATOM | 1675 | CE2 | PHE | 114 | 6.078 | -2.512 | -16.327 | 1.00 | 0.26 |
| ATOM | 1676 | HE2 | PHE | 114 | 5.511 | -2.273 | -17.214 | 1.00 | 0.30 |
| ATOM | 1677 | CZ | PHE | 114 | 6.168 | -3.839 | -15.890 | 1.00 | 0.32 |
| ATOM | 1678 | HZ | PHE | 114 | 5.670 | -4.623 | -16.438 | 1.00 | 0.35 |
| ATOM | 1679 | C | PHE | 114 | 6.900 | -1.452 | -11.676 | 1.00 | 0.17 |
| ATOM | 1680 | O | PHE | 114 | 5.842 | -2.034 | -11.806 | 1.00 | 0.17 |
| ATOM | 1681 | N | LEU | 115 | 7.774 | -1.846 | -10.797 | 1.00 | 0.18 |
| ATOM | 1682 | HN | LEU | 115 | 8.631 | -1.380 | -10.706 | 1.00 | 0.18 |
| ATOM | 1683 | CA | LEU | 115 | 7.463 | -3.028 | -9.946 | 1.00 | 0.20 |
| ATOM | 1684 | HA | LEU | 115 | 7.297 | -3.882 | -10.579 | 1.00 | 0.21 |
| ATOM | 1685 | CB | LEU | 115 | 8.634 | -3.304 | -8.984 | 1.00 | 0.23 |
| ATOM | 1686 | HB1 | LEU | 115 | 8.237 | -3.650 | -8.041 | 1.00 | 0.26 |
| ATOM | 1687 | HB2 | LEU | 115 | 9.172 | -2.387 | -8.821 | 1.00 | 0.22 |
| ATOM | 1688 | CG | LEU | 115 | 9.612 | -4.369 | -9.539 | 1.00 | 0.28 |
| ATOM | 1689 | HG | LEU | 115 | 10.397 | -4.525 | -8.812 | 1.00 | 0.33 |
| ATOM | 1690 | CD1 | LEU | 115 | 8.886 | -5.702 | -9.749 | 1.00 | 0.36 |
| ATOM | 1691 | HD11 | LEU | 115 | 9.551 | -6.514 | -9.498 | 1.00 | 0.99 |
| ATOM | 1692 | HD12 | LEU | 115 | 8.578 | -5.795 | -10.779 | 1.00 | 1.11 |
| ATOM | 1693 | HD13 | LEU | 115 | 8.017 | -5.740 | -9.109 | 1.00 | 1.13 |
| ATOM | 1694 | CD2 | LEU | 115 | 10.249 | -3.903 | -10.859 | 1.00 | 0.30 |
| ATOM | 1695 | HD21 | LEU | 115 | 10.497 | -4.761 | -11.466 | 1.00 | 1.10 |
| ATOM | 1696 | HD22 | LEU | 115 | 11.149 | -3.351 | -10.645 | 1.00 | 1.06 |
| ATOM | 1697 | HD23 | LEU | 115 | 9.567 | -3.272 | -11.395 | 1.00 | 1.01 |
| ATOM | 1698 | C | LEU | 115 | 6.194 | -2.748 | -9.136 | 1.00 | 0.19 |
| ATOM | 1699 | O | LEU | 115 | 5.280 | -3.548 | -9.106 | 1.00 | 0.20 |
| ATOM | 1700 | N | VAL | 116 | 6.130 | -1.624 | -8.475 | 1.00 | 0.18 |
| ATOM | 1701 | HN | VAL | 116 | 6.879 | -0.993 | -8.508 | 1.00 | 0.18 |
| ATOM | 1702 | CA | VAL | 116 | 4.919 | -1.305 | -7.664 | 1.00 | 0.19 |
| ATOM | 1703 | HA | VAL | 116 | 4.686 | -2.146 | -7.028 | 1.00 | 0.21 |
| ATOM | 1704 | CB | VAL | 116 | 5.203 | -0.078 | -6.794 | 1.00 | 0.20 |
| ATOM | 1705 | HB | VAL | 116 | 5.581 | 0.722 | -7.414 | 1.00 | 0.19 |
| ATOM | 1706 | CG1 | VAL | 116 | 3.914 | 0.381 | -6.103 | 1.00 | 0.22 |
| ATOM | 1707 | HG11 | VAL | 116 | 3.253 | 0.832 | -6.828 | 1.00 | 1.05 |
| ATOM | 1708 | HG12 | VAL | 116 | 4.155 | 1.105 | -5.339 | 1.00 | 1.05 |
| ATOM | 1709 | HG13 | VAL | 116 | 3.426 | -0.470 | -5.650 | 1.00 | 1.03 |
| ATOM | 1710 | CG2 | VAL | 116 | 6.246 | -0.443 | -5.737 | 1.00 | 0.21 |
| ATOM | 1711 | HG21 | VAL | 116 | 7.188 | -0.654 | -6.221 | 1.00 | 1.02 |
| ATOM | 1712 | HG22 | VAL | 116 | 5.917 | -1.317 | -5.194 | 1.00 | 0.98 |
| ATOM | 1713 | HG23 | VAL | 116 | 6.370 | 0.382 | -5.052 | 1.00 | 1.03 |
| ATOM | 1714 | C | VAL | 116 | 3.724 | -1.020 | -8.582 | 1.00 | 0.18 |
| ATOM | 1715 | O | VAL | 116 | 2.615 | -1.433 | -8.312 | 1.00 | 0.19 |
| ATOM | 1716 | N | ALA | 117 | 3.934 | -0.307 | -9.659 | 1.00 | 0.17 |
| ATOM | 1717 | HN | ALA | 117 | 4.833 | 0.028 | -9.859 | 1.00 | 0.16 |
| ATOM | 1718 | CA | ALA | 117 | 2.796 | 0.007 | -10.572 | 1.00 | 0.17 |
| ATOM | 1719 | HA | ALA | 117 | 2.064 | 0.598 | -10.044 | 1.00 | 0.19 |
| ATOM | 1720 | CB | ALA | 117 | 3.306 | 0.795 | -11.780 | 1.00 | 0.18 |
| ATOM | 1721 | HB1 | ALA | 117 | 4.378 | 0.709 | -11.840 | 1.00 | 1.05 |
| ATOM | 1722 | HB2 | ALA | 117 | 3.033 | 1.834 | -11.674 | 1.00 | 1.01 |
| ATOM | 1723 | HB3 | ALA | 117 | 2.863 | 0.397 | -12.682 | 1.00 | 0.98 |
| ATOM | 1724 | C | ALA | 117 | 2.150 | -1.291 | -11.058 | 1.00 | 0.17 |
| ATOM | 1725 | O | ALA | 117 | 0.956 | -1.480 | -10.951 | 1.00 | 0.19 |
| ATOM | 1726 | N | ALA | 118 | 2.931 | -2.187 | -11.588 | 1.00 | 0.16 |
| ATOM | 1727 | HN | ALA | 118 | 3.893 | -2.015 | -11.663 | 1.00 | 0.16 |
| ATOM | 1728 | CA | ALA | 118 | 2.366 | -3.472 | -12.083 | 1.00 | 0.17 |
| ATOM | 1729 | HA | ALA | 118 | 1.643 | -3.273 | -12.859 | 1.00 | 0.19 |
| ATOM | 1730 | CB | ALA | 118 | 3.491 | -4.335 | -12.653 | 1.00 | 0.17 |
| ATOM | 1731 | HB1 | ALA | 118 | 3.125 | -5.338 | -12.812 | 1.00 | 1.05 |
| ATOM | 1732 | HB2 | ALA | 118 | 4.316 | -4.358 | -11.956 | 1.00 | 1.02 |
| ATOM | 1733 | HB3 | ALA | 118 | 3.824 | -3.824 | -12.582 | 1.00 | 1.02 |

27/75

| | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|---------|------|------|
| ATOM | 1734 | C | ALA | 118 | 1.687 | -4.220 | -10.935 | 1.00 | 0.17 |
| ATOM | 1735 | O | ALA | 118 | 0.699 | -4.901 | -11.124 | 1.00 | 0.18 |
| ATOM | 1736 | N | HIS | 119 | 2.225 | -4.123 | -9.751 | 1.00 | 0.16 |
| ATOM | 1737 | HN | HIS | 119 | 3.035 | -3.585 | -9.623 | 1.00 | 0.16 |
| ATOM | 1738 | CA | HIS | 119 | 1.627 | -4.855 | -8.599 | 1.00 | 0.17 |
| ATOM | 1739 | HA | HIS | 119 | 1.576 | -5.907 | -8.833 | 1.00 | 0.18 |
| ATOM | 1740 | CB | HIS | 119 | 2.513 | -4.655 | -7.368 | 1.00 | 0.19 |
| ATOM | 1741 | HB1 | HIS | 119 | 2.547 | -3.605 | -7.116 | 1.00 | 0.19 |
| ATOM | 1742 | HB2 | HIS | 119 | 3.512 | -5.005 | -7.584 | 1.00 | 0.20 |
| ATOM | 1743 | CG | HIS | 119 | 1.950 | -5.431 | -6.210 | 1.00 | 0.21 |
| ATOM | 1744 | ND1 | HIS | 119 | 2.228 | -6.775 | -6.020 | 1.00 | 0.26 |
| ATOM | 1745 | HD1 | HIS | 119 | 2.791 | -7.336 | -6.593 | 1.00 | 0.30 |
| ATOM | 1746 | CD2 | HIS | 119 | 1.128 | -5.067 | -5.172 | 1.00 | 0.20 |
| ATOM | 1747 | HD2 | HIS | 119 | 0.719 | -4.079 | -5.019 | 1.00 | 0.21 |
| ATOM | 1748 | CE1 | HIS | 119 | 1.585 | -7.168 | -4.906 | 1.00 | 0.27 |
| ATOM | 1749 | HE1 | HIS | 119 | 1.622 | -8.171 | -4.509 | 1.00 | 0.33 |
| ATOM | 1750 | NE2 | HIS | 119 | 0.899 | -6.166 | -4.350 | 1.00 | 0.23 |
| ATOM | 1751 | C | HIS | 119 | 0.215 | -4.333 | -8.299 | 1.00 | 0.17 |
| ATOM | 1752 | O | HIS | 119 | -0.721 | -5.101 | -8.185 | 1.00 | 0.18 |
| ATOM | 1753 | N | GLU | 120 | 0.043 | -3.044 | -8.160 | 1.00 | 0.18 |
| ATOM | 1754 | HN | GLU | 120 | 0.801 | -2.430 | -8.248 | 1.00 | 0.18 |
| ATOM | 1755 | CA | GLU | 120 | -1.322 | -2.520 | -7.860 | 1.00 | 0.20 |
| ATOM | 1756 | HA | GLU | 120 | -1.666 | -2.977 | -6.943 | 1.00 | 0.21 |
| ATOM | 1757 | CB | GLU | 120 | -1.294 | -0.999 | -7.668 | 1.00 | 0.22 |
| ATOM | 1758 | HB1 | GLU | 120 | -0.719 | -0.763 | -6.785 | 1.00 | 0.37 |
| ATOM | 1759 | HB2 | GLU | 120 | -2.302 | -0.635 | -7.542 | 1.00 | 0.33 |
| ATOM | 1760 | CG | GLU | 120 | -0.663 | -0.314 | -8.875 | 1.00 | 0.41 |
| ATOM | 1761 | HG1 | GLU | 120 | -1.125 | -0.668 | -9.781 | 1.00 | 0.63 |
| ATOM | 1762 | HG2 | GLU | 120 | 0.393 | -0.531 | -8.895 | 1.00 | 0.87 |
| ATOM | 1763 | CD | GLU | 120 | -0.875 | 1.194 | -8.757 | 1.00 | 0.94 |
| ATOM | 1764 | OE1 | GLU | 120 | -0.757 | 1.703 | -7.654 | 1.00 | 1.67 |
| ATOM | 1765 | OE2 | GLU | 120 | -1.151 | 1.816 | -9.769 | 1.00 | 1.56 |
| ATOM | 1766 | C | GLU | 120 | -2.291 | -2.903 | -8.984 | 1.00 | 0.20 |
| ATOM | 1767 | O | GLU | 120 | -3.432 | -3.238 | -8.737 | 1.00 | 0.21 |
| ATOM | 1768 | N | PHE | 121 | -1.853 | -2.872 | -10.217 | 1.00 | 0.19 |
| ATOM | 1769 | HN | PHE | 121 | -0.928 | -2.608 | -10.405 | 1.00 | 0.19 |
| ATOM | 1770 | CA | PHE | 121 | -2.767 | -3.251 | -11.331 | 1.00 | 0.21 |
| ATOM | 1771 | HA | PHE | 121 | -3.628 | -2.600 | -11.317 | 1.00 | 0.23 |
| ATOM | 1772 | CB | PHE | 121 | -2.053 | -3.130 | -12.685 | 1.00 | 0.22 |
| ATOM | 1773 | HB1 | PHE | 121 | -2.576 | -3.726 | -13.419 | 1.00 | 0.24 |
| ATOM | 1774 | HB2 | PHE | 121 | -1.041 | -3.493 | -12.587 | 1.00 | 0.21 |
| ATOM | 1775 | CG | PHE | 121 | -2.026 | -1.684 | -13.141 | 1.00 | 0.25 |
| ATOM | 1776 | CD1 | PHE | 121 | -0.804 | -1.019 | -13.308 | 1.00 | 0.27 |
| ATOM | 1777 | HD1 | PHE | 121 | 0.121 | -1.535 | -13.113 | 1.00 | 0.40 |
| ATOM | 1778 | CD2 | PHE | 121 | -3.227 | -1.007 | -13.403 | 1.00 | 0.45 |
| ATOM | 1779 | HD2 | PHE | 121 | -4.173 | -1.513 | -13.281 | 1.00 | 0.60 |
| ATOM | 1780 | CE1 | PHE | 121 | -0.781 | 0.314 | -13.733 | 1.00 | 0.29 |
| ATOM | 1781 | HE1 | PHE | 121 | 0.163 | 0.824 | -13.862 | 1.00 | 0.39 |
| ATOM | 1782 | CE2 | PHE | 121 | -3.202 | 0.327 | -13.828 | 1.00 | 0.49 |
| ATOM | 1783 | HE2 | PHE | 121 | -4.127 | 0.847 | -14.029 | 1.00 | 0.68 |
| ATOM | 1784 | CZ | PHE | 121 | -1.979 | 0.988 | -13.993 | 1.00 | 0.34 |
| ATOM | 1785 | HZ | PHE | 121 | -1.961 | 2.017 | -14.321 | 1.00 | 0.38 |
| ATOM | 1786 | C | PHE | 121 | -3.228 | -4.693 | -11.120 | 1.00 | 0.20 |
| ATOM | 1787 | O | PHE | 121 | -4.374 | -5.027 | -11.344 | 1.00 | 0.21 |
| ATOM | 1788 | N | GLY | 122 | -2.344 | -5.551 | -10.690 | 1.00 | 0.18 |
| ATOM | 1789 | HN | GLY | 122 | -1.424 | -5.262 | -10.514 | 1.00 | 0.17 |
| ATOM | 1790 | CA | GLY | 122 | -2.737 | -6.970 | -10.464 | 1.00 | 0.20 |
| ATOM | 1791 | HA1 | GLY | 122 | -1.890 | -7.523 | -10.092 | 1.00 | 0.21 |
| ATOM | 1792 | HA2 | GLY | 122 | -3.072 | -7.404 | -11.394 | 1.00 | 0.21 |
| ATOM | 1793 | C | GLY | 122 | -3.867 | -7.022 | -9.435 | 1.00 | 0.20 |
| ATOM | 1794 | O | GLY | 122 | -4.823 | -7.756 | -9.589 | 1.00 | 0.22 |
| ATOM | 1795 | N | HIS | 123 | -3.778 | -6.240 | -8.392 | 1.00 | 0.20 |
| ATOM | 1796 | HN | HIS | 123 | -3.005 | -5.644 | -8.287 | 1.00 | 0.20 |
| ATOM | 1797 | CA | HIS | 123 | -4.864 | -6.243 | -7.371 | 1.00 | 0.22 |
| ATOM | 1798 | HA | HIS | 123 | -5.047 | -7.255 | -7.042 | 1.00 | 0.23 |
| ATOM | 1799 | CB | HIS | 123 | -4.456 | -5.382 | -6.174 | 1.00 | 0.25 |
| ATOM | 1800 | HB1 | HIS | 123 | -5.324 | -5.180 | -5.564 | 1.00 | 0.30 |
| ATOM | 1801 | HB2 | HIS | 123 | -4.041 | -4.449 | -6.527 | 1.00 | 0.25 |
| ATOM | 1802 | CG | HIS | 123 | -3.427 | -6.108 | -5.354 | 1.00 | 0.27 |
| ATOM | 1803 | ND1 | HIS | 123 | -3.736 | -7.247 | -4.628 | 1.00 | 0.37 |
| ATOM | 1804 | HD1 | HIS | 123 | -4.611 | -7.685 | -4.581 | 1.00 | 0.45 |
| ATOM | 1805 | CD2 | HIS | 123 | -2.096 | -5.866 | -5.125 | 1.00 | 0.25 |
| ATOM | 1806 | HD2 | HIS | 123 | -1.532 | -5.046 | -5.545 | 1.00 | 0.27 |
| ATOM | 1807 | CE1 | HIS | 123 | -2.614 | -7.644 | -4.001 | 1.00 | 0.38 |
| ATOM | 1808 | HE1 | HIS | 123 | -2.553 | -8.514 | -3.367 | 1.00 | 0.47 |
| ATOM | 1809 | NE2 | HIS | 123 | -1.584 | -6.837 | -4.269 | 1.00 | 0.29 |
| ATOM | 1810 | C | HIS | 123 | -6.137 | -5.671 | -7.883 | 1.00 | 0.22 |

28/75

| | | | | | | | | | |
|------|------|------|-----|-----|--------|---------|---------|------|------|
| ATOM | 1811 | O | HIS | 123 | -7.229 | -6.148 | -7.755 | 1.00 | 0.25 |
| ATOM | 1812 | N | SER | 124 | -6.002 | -4.646 | -8.788 | 1.00 | 0.23 |
| ATOM | 1813 | HN | SER | 124 | -5.110 | -4.278 | -8.962 | 1.00 | 0.22 |
| ATOM | 1814 | CA | SER | 124 | -7.196 | -4.030 | -9.429 | 1.00 | 0.25 |
| ATOM | 1815 | HA | SER | 124 | -7.928 | -3.790 | -8.672 | 1.00 | 0.27 |
| ATOM | 1816 | CB | SER | 124 | -6.778 | -2.751 | -10.156 | 1.00 | 0.27 |
| ATOM | 1817 | HB1 | SER | 124 | -6.219 | -2.119 | -9.478 | 1.00 | 0.29 |
| ATOM | 1818 | HB2 | SER | 124 | -7.654 | -2.224 | -10.494 | 1.00 | 0.29 |
| ATOM | 1819 | OG | SER | 124 | -5.975 | -3.091 | -11.279 | 1.00 | 0.25 |
| ATOM | 1820 | HG | SER | 124 | -6.545 | -3.131 | -12.050 | 1.00 | 0.88 |
| ATOM | 1821 | C | SER | 124 | -7.805 | -5.006 | -10.437 | 1.00 | 0.24 |
| ATOM | 1822 | O | SER | 124 | -8.975 | -4.932 | -10.755 | 1.00 | 0.26 |
| ATOM | 1823 | N | LEU | 125 | -7.022 | -5.913 | -10.952 | 1.00 | 0.22 |
| ATOM | 1824 | HN | LEU | 125 | -6.078 | -5.953 | -10.690 | 1.00 | 0.21 |
| ATOM | 1825 | CA | LEU | 125 | -7.562 | -6.879 | -11.949 | 1.00 | 0.23 |
| ATOM | 1826 | HA | LEU | 125 | -8.285 | -6.374 | -12.568 | 1.00 | 0.24 |
| ATOM | 1827 | CB | LEU | 125 | -6.420 | -7.398 | -12.827 | 1.00 | 0.22 |
| ATOM | 1828 | HB1 | LEU | 125 | -6.759 | -8.247 | -13.398 | 1.00 | 0.24 |
| ATOM | 1829 | HB2 | LEU | 125 | -5.594 | -7.698 | -12.197 | 1.00 | 0.22 |
| ATOM | 1830 | CG | LEU | 125 | -5.956 | -6.280 | -13.779 | 1.00 | 0.22 |
| ATOM | 1831 | HG | LEU | 125 | -5.928 | -5.343 | -13.241 | 1.00 | 0.24 |
| ATOM | 1832 | CD1 | LEU | 125 | -4.556 | -6.601 | -14.302 | 1.00 | 0.25 |
| ATOM | 1833 | HD11 | LEU | 125 | -4.588 | -7.515 | -14.874 | 1.00 | 0.99 |
| ATOM | 1834 | HD12 | LEU | 125 | -3.879 | -6.719 | -13.471 | 1.00 | 1.00 |
| ATOM | 1835 | HD13 | LEU | 125 | -4.215 | -5.794 | -14.933 | 1.00 | 1.05 |
| ATOM | 1836 | CD2 | LEU | 125 | -6.913 | -6.155 | -14.976 | 1.00 | 0.24 |
| ATOM | 1837 | HD21 | LEU | 125 | -7.793 | -5.604 | -14.682 | 1.00 | 1.05 |
| ATOM | 1838 | HD22 | LEU | 125 | -7.201 | -7.135 | -15.324 | 1.00 | 1.00 |
| ATOM | 1839 | HD23 | LEU | 125 | -6.415 | -5.627 | -15.775 | 1.00 | 1.03 |
| ATOM | 1840 | C | LEU | 125 | -8.256 | -8.044 | -11.234 | 1.00 | 0.24 |
| ATOM | 1841 | O | LEU | 125 | -8.790 | -8.935 | -11.864 | 1.00 | 0.33 |
| ATOM | 1842 | N | GLY | 126 | -8.277 | -8.035 | -9.927 | 1.00 | 0.24 |
| ATOM | 1843 | HN | GLY | 126 | -7.858 | -7.298 | -9.435 | 1.00 | 0.29 |
| ATOM | 1844 | CA | GLY | 126 | -8.968 | -9.132 | -9.185 | 1.00 | 0.27 |
| ATOM | 1845 | HA1 | GLY | 126 | -9.748 | -9.545 | -9.807 | 1.00 | 0.29 |
| ATOM | 1846 | HA2 | GLY | 126 | -9.408 | -8.727 | -8.285 | 1.00 | 0.29 |
| ATOM | 1847 | C | GLY | 126 | -7.985 | -10.245 | -8.809 | 1.00 | 0.26 |
| ATOM | 1848 | O | GLY | 126 | -8.377 | -11.268 | -8.283 | 1.00 | 0.30 |
| ATOM | 1849 | N | LEU | 127 | -6.719 | -10.068 | -9.063 | 1.00 | 0.23 |
| ATOM | 1850 | HN | LEU | 127 | -6.410 | -9.239 | -9.484 | 1.00 | 0.22 |
| ATOM | 1851 | CA | LEU | 127 | -5.744 | -11.138 | -8.700 | 1.00 | 0.25 |
| ATOM | 1852 | HA | LEU | 127 | -6.212 | -12.099 | -8.815 | 1.00 | 0.28 |
| ATOM | 1853 | CB | LEU | 127 | -4.507 | -11.052 | -9.602 | 1.00 | 0.23 |
| ATOM | 1854 | HB1 | LEU | 127 | -3.733 | -11.696 | -9.211 | 1.00 | 0.25 |
| ATOM | 1855 | HB2 | LEU | 127 | -4.156 | -10.033 | -9.602 | 1.00 | 0.22 |
| ATOM | 1856 | CG | LEU | 127 | -4.844 | -11.471 | -11.045 | 1.00 | 0.24 |
| ATOM | 1857 | HG | LEU | 127 | -5.707 | -10.915 | -11.384 | 1.00 | 0.23 |
| ATOM | 1858 | CD1 | LEU | 127 | -3.646 | -11.159 | -11.962 | 1.00 | 0.24 |
| ATOM | 1859 | HD11 | LEU | 127 | -4.001 | -10.692 | -12.868 | 1.00 | 1.00 |
| ATOM | 1860 | HD12 | LEU | 127 | -3.126 | -12.073 | -12.208 | 1.00 | 1.02 |
| ATOM | 1861 | HD13 | LEU | 127 | -2.962 | -10.491 | -11.460 | 1.00 | 1.03 |
| ATOM | 1862 | CD2 | LEU | 127 | -5.150 | -12.980 | -11.109 | 1.00 | 0.30 |
| ATOM | 1863 | HD21 | LEU | 127 | -5.021 | -13.334 | -12.121 | 1.00 | 1.04 |
| ATOM | 1864 | HD22 | LEU | 127 | -6.169 | -13.159 | -10.805 | 1.00 | 1.11 |
| ATOM | 1865 | HD23 | LEU | 127 | -4.478 | -13.515 | -10.454 | 1.00 | 1.03 |
| ATOM | 1866 | C | LEU | 127 | -5.315 | -10.969 | -7.241 | 1.00 | 0.28 |
| ATOM | 1867 | O | LEU | 127 | -5.245 | -9.872 | -6.723 | 1.00 | 0.32 |
| ATOM | 1868 | N | ASP | 128 | -5.027 | -12.059 | -6.581 | 1.00 | 0.32 |
| ATOM | 1869 | HN | ASP | 128 | -5.093 | -12.928 | -7.029 | 1.00 | 0.34 |
| ATOM | 1870 | CA | ASP | 128 | -4.598 | -11.997 | -5.154 | 1.00 | 0.39 |
| ATOM | 1871 | HA | ASP | 128 | -4.882 | -11.046 | -4.728 | 1.00 | 0.40 |
| ATOM | 1872 | CB | ASP | 128 | -5.271 | -13.130 | -4.375 | 1.00 | 0.48 |
| ATOM | 1873 | HB1 | ASP | 128 | -4.779 | -14.064 | -4.600 | 1.00 | 0.48 |
| ATOM | 1874 | HB2 | ASP | 128 | -6.311 | -13.193 | -4.661 | 1.00 | 0.50 |
| ATOM | 1875 | CG | ASP | 128 | -5.171 | -12.854 | -2.873 | 1.00 | 0.55 |
| ATOM | 1876 | OD1 | ASP | 128 | -4.082 | -12.980 | -2.339 | 1.00 | 1.23 |
| ATOM | 1877 | OD2 | ASP | 128 | -6.185 | -12.521 | -2.283 | 1.00 | 1.22 |
| ATOM | 1878 | C | ASP | 128 | -3.078 | -12.159 | -5.082 | 1.00 | 0.37 |
| ATOM | 1879 | O | ASP | 128 | -2.424 | -12.387 | -6.080 | 1.00 | 0.59 |
| ATOM | 1880 | N | HIS | 129 | -2.507 | -12.042 | -3.914 | 1.00 | 0.23 |
| ATOM | 1881 | HN | HIS | 129 | -3.048 | -11.856 | -3.118 | 1.00 | 0.32 |
| ATOM | 1882 | CA | HIS | 129 | -1.029 | -12.189 | -3.797 | 1.00 | 0.22 |
| ATOM | 1883 | HA | HIS | 129 | -0.543 | -11.439 | -4.401 | 1.00 | 0.21 |
| ATOM | 1884 | CB | HIS | 129 | -0.606 | -12.019 | -2.335 | 1.00 | 0.23 |
| ATOM | 1885 | HB1 | HIS | 129 | 0.430 | -12.302 | -2.227 | 1.00 | 0.24 |
| ATOM | 1886 | HB2 | HIS | 129 | -1.217 | -12.653 | -1.710 | 1.00 | 0.25 |
| ATOM | 1887 | CG | HIS | 129 | -0.779 | -10.585 | -1.912 | 1.00 | 0.22 |

29/75

| | | | | | | | | | |
|------|------|-----|-----|-----|--------|---------|---------|------|------|
| ATOM | 1888 | ND1 | HIS | 129 | -1.862 | -10.161 | -1.156 | 1.00 | 0.35 |
| ATOM | 1889 | HD1 | HIS | 129 | -2.602 | -10.720 | -0.841 | 1.00 | 0.53 |
| ATOM | 1890 | CD2 | HIS | 129 | -0.007 | -9.468 | -2.118 | 1.00 | 0.34 |
| ATOM | 1891 | HD2 | HIS | 129 | 0.918 | -9.447 | -2.673 | 1.00 | 0.54 |
| ATOM | 1892 | CE1 | HIS | 129 | -1.711 | -8.842 | -0.936 | 1.00 | 0.31 |
| ATOM | 1893 | HE1 | HIS | 129 | -2.406 | -8.239 | -0.370 | 1.00 | 0.44 |
| ATOM | 1894 | NE2 | HIS | 129 | -0.597 | -8.369 | -1.501 | 1.00 | 0.28 |
| ATOM | 1895 | C | HIS | 129 | -0.614 | -13.584 | -4.277 | 1.00 | 0.24 |
| ATOM | 1896 | O | HIS | 129 | -1.267 | -14.568 | -3.991 | 1.00 | 0.28 |
| ATOM | 1897 | N | SER | 130 | 0.474 | -13.671 | -4.999 | 1.00 | 0.24 |
| ATOM | 1898 | HN | SER | 130 | 0.984 | -12.862 | -5.210 | 1.00 | 0.23 |
| ATOM | 1899 | CA | SER | 130 | 0.949 | -14.996 | -5.498 | 1.00 | 0.29 |
| ATOM | 1900 | HA | SER | 130 | 0.139 | -15.710 | -5.464 | 1.00 | 0.33 |
| ATOM | 1901 | CB | SER | 130 | 1.442 | -14.852 | -6.938 | 1.00 | 0.32 |
| ATOM | 1902 | HB1 | SER | 130 | 2.201 | -14.082 | -6.982 | 1.00 | 0.31 |
| ATOM | 1903 | HB2 | SER | 130 | 0.618 | -14.577 | -7.576 | 1.00 | 0.35 |
| ATOM | 1904 | OG | SER | 130 | 1.980 | -16.092 | -7.378 | 1.00 | 0.40 |
| ATOM | 1905 | HG | SER | 130 | 1.254 | -16.714 | -7.469 | 1.00 | 0.97 |
| ATOM | 1906 | C | SER | 130 | 2.096 | -15.484 | -4.609 | 1.00 | 0.28 |
| ATOM | 1907 | O | SER | 130 | 2.801 | -14.696 | -4.009 | 1.00 | 0.29 |
| ATOM | 1908 | N | LYS | 131 | 2.287 | -16.775 | -4.514 | 1.00 | 0.30 |
| ATOM | 1909 | HN | LYS | 131 | 1.705 | -17.393 | -5.003 | 1.00 | 0.32 |
| ATOM | 1910 | CA | LYS | 131 | 3.386 | -17.310 | -3.656 | 1.00 | 0.32 |
| ATOM | 1911 | HA | LYS | 131 | 3.665 | -16.567 | -2.923 | 1.00 | 0.34 |
| ATOM | 1912 | CB | LYS | 131 | 2.903 | -18.572 | -2.936 | 1.00 | 0.39 |
| ATOM | 1913 | HB1 | LYS | 131 | 3.714 | -18.988 | -2.355 | 1.00 | 0.42 |
| ATOM | 1914 | HB2 | LYS | 131 | 2.572 | -19.298 | -3.664 | 1.00 | 0.40 |
| ATOM | 1915 | CG | LYS | 131 | 1.743 | -18.214 | -2.003 | 1.00 | 0.45 |
| ATOM | 1916 | HG1 | LYS | 131 | 0.932 | -17.798 | -2.581 | 1.00 | 0.79 |
| ATOM | 1917 | HG2 | LYS | 131 | 2.077 | -17.488 | -1.276 | 1.00 | 1.01 |
| ATOM | 1918 | CD | LYS | 131 | 1.255 | -19.472 | -1.280 | 1.00 | 1.18 |
| ATOM | 1919 | HD1 | LYS | 131 | 2.064 | -19.890 | -0.698 | 1.00 | 1.86 |
| ATOM | 1920 | HD2 | LYS | 131 | 0.921 | -20.199 | -2.006 | 1.00 | 1.66 |
| ATOM | 1921 | CE | LYS | 131 | 0.096 | -19.108 | -0.349 | 1.00 | 1.52 |
| ATOM | 1922 | HE1 | LYS | 131 | -0.788 | -18.908 | -0.937 | 1.00 | 1.92 |
| ATOM | 1923 | HE2 | LYS | 131 | 0.355 | -18.229 | 0.222 | 1.00 | 1.93 |
| ATOM | 1924 | NZ | LYS | 131 | -0.174 | -20.242 | 0.581 | 1.00 | 2.23 |
| ATOM | 1925 | HZ1 | LYS | 131 | -1.103 | -20.109 | 1.030 | 1.00 | 2.72 |
| ATOM | 1926 | HZ2 | LYS | 131 | 0.565 | -20.272 | 1.313 | 1.00 | 2.53 |
| ATOM | 1927 | HZ3 | LYS | 131 | -0.174 | -21.135 | 0.050 | 1.00 | 2.72 |
| ATOM | 1928 | C | LYS | 131 | 4.604 | -17.649 | -4.521 | 1.00 | 0.31 |
| ATOM | 1929 | O | LYS | 131 | 5.612 | -18.116 | -4.027 | 1.00 | 0.34 |
| ATOM | 1930 | N | ASP | 132 | 4.532 | -17.411 | -5.804 | 1.00 | 0.29 |
| ATOM | 1931 | HN | ASP | 132 | 3.717 | -17.028 | -6.190 | 1.00 | 0.28 |
| ATOM | 1932 | CA | ASP | 132 | 5.703 | -17.719 | -6.674 | 1.00 | 0.30 |
| ATOM | 1933 | HA | ASP | 132 | 6.187 | -18.601 | -6.302 | 1.00 | 0.32 |
| ATOM | 1934 | CB | ASP | 132 | 5.225 | -17.970 | -8.108 | 1.00 | 0.32 |
| ATOM | 1935 | HB1 | ASP | 132 | 4.727 | -17.090 | -8.483 | 1.00 | 0.31 |
| ATOM | 1936 | HB2 | ASP | 132 | 4.539 | -18.804 | -8.118 | 1.00 | 0.34 |
| ATOM | 1937 | CG | ASP | 132 | 6.430 | -18.289 | -8.996 | 1.00 | 0.35 |
| ATOM | 1938 | OD1 | ASP | 132 | 6.457 | -19.371 | -9.558 | 1.00 | 1.10 |
| ATOM | 1939 | OD2 | ASP | 132 | 7.306 | -17.446 | -9.097 | 1.00 | 1.15 |
| ATOM | 1940 | C | ASP | 132 | 6.656 | -16.501 | -6.659 | 1.00 | 0.28 |
| ATOM | 1941 | O | ASP | 132 | 6.226 | -15.399 | -6.939 | 1.00 | 0.28 |
| ATOM | 1942 | N | PRO | 133 | 7.930 | -16.658 | -6.328 | 1.00 | 0.30 |
| ATOM | 1943 | CA | PRO | 133 | 8.852 | -15.484 | -6.296 | 1.00 | 0.31 |
| ATOM | 1944 | HA | PRO | 133 | 8.517 | -14.766 | -5.566 | 1.00 | 0.32 |
| ATOM | 1945 | CB | PRO | 133 | 10.173 | -16.097 | -5.832 | 1.00 | 0.36 |
| ATOM | 1946 | HB1 | PRO | 133 | 10.441 | -15.694 | -4.867 | 1.00 | 0.36 |
| ATOM | 1947 | HB2 | PRO | 133 | 10.949 | -15.869 | -6.549 | 1.00 | 0.41 |
| ATOM | 1948 | CG | PRO | 133 | 10.007 | -17.615 | -5.721 | 1.00 | 0.42 |
| ATOM | 1949 | HG1 | PRO | 133 | 10.293 | -17.940 | -4.732 | 1.00 | 0.51 |
| ATOM | 1950 | HG2 | PRO | 133 | 10.630 | -18.103 | -6.457 | 1.00 | 0.51 |
| ATOM | 1951 | CD | PRO | 133 | 8.540 | -17.972 | -5.969 | 1.00 | 0.35 |
| ATOM | 1952 | HD2 | PRO | 133 | 8.456 | -18.679 | -6.785 | 1.00 | 0.34 |
| ATOM | 1953 | HD1 | PRO | 133 | 8.091 | -18.362 | -5.069 | 1.00 | 0.38 |
| ATOM | 1954 | C | PRO | 133 | 9.032 | -14.810 | -7.662 | 1.00 | 0.31 |
| ATOM | 1955 | O | PRO | 133 | 9.496 | -13.691 | -7.749 | 1.00 | 0.34 |
| ATOM | 1956 | N | GLY | 134 | 8.684 | -15.477 | -8.729 | 1.00 | 0.32 |
| ATOM | 1957 | HN | GLY | 134 | 8.320 | -16.382 | -8.647 | 1.00 | 0.35 |
| ATOM | 1958 | CA | GLY | 134 | 8.860 | -14.856 | -10.074 | 1.00 | 0.34 |
| ATOM | 1959 | HA1 | GLY | 134 | 9.048 | -15.630 | -10.803 | 1.00 | 0.37 |
| ATOM | 1960 | HA2 | GLY | 134 | 9.701 | -14.177 | -10.047 | 1.00 | 0.36 |
| ATOM | 1961 | C | GLY | 134 | 7.598 | -14.087 | -10.471 | 1.00 | 0.29 |
| ATOM | 1962 | O | GLY | 134 | 7.563 | -13.420 | -11.486 | 1.00 | 0.29 |
| ATOM | 1963 | N | ALA | 135 | 6.563 | -14.168 | -9.683 | 1.00 | 0.27 |
| ATOM | 1964 | HN | ALA | 135 | 6.607 | -14.709 | -8.867 | 1.00 | 0.28 |

30/75

| | | | | | | | | | |
|------|------|------|-----|-----|--------|---------|---------|------|------|
| ATOM | 1965 | CA | ALA | 135 | 5.312 | -13.434 | -10.026 | 1.00 | 0.24 |
| ATOM | 1966 | HA | ALA | 135 | 5.199 | -13.401 | -11.099 | 1.00 | 0.25 |
| ATOM | 1967 | CB | ALA | 135 | 4.109 | -14.151 | -9.410 | 1.00 | 0.25 |
| ATOM | 1968 | HB1 | ALA | 135 | 3.633 | -14.765 | -10.160 | 1.00 | 1.07 |
| ATOM | 1969 | HB2 | ALA | 135 | 3.405 | -13.421 | -9.041 | 1.00 | 1.01 |
| ATOM | 1970 | HB3 | ALA | 135 | 4.442 | -14.774 | -8.593 | 1.00 | 1.04 |
| ATOM | 1971 | C | ALA | 135 | 5.388 | -12.007 | -9.479 | 1.00 | 0.21 |
| ATOM | 1972 | O | ALA | 135 | 5.968 | -11.760 | -8.440 | 1.00 | 0.23 |
| ATOM | 1973 | N | LEU | 136 | 4.799 | -11.067 | -10.164 | 1.00 | 0.22 |
| ATOM | 1974 | HN | LEU | 136 | 4.330 | -11.286 | -10.996 | 1.00 | 0.24 |
| ATOM | 1975 | CA | LEU | 136 | 4.830 | -9.660 | -9.676 | 1.00 | 0.23 |
| ATOM | 1976 | HA | LEU | 136 | 5.842 | -9.382 | -9.427 | 1.00 | 0.25 |
| ATOM | 1977 | CB | LEU | 136 | 4.279 | -8.724 | -10.761 | 1.00 | 0.25 |
| ATOM | 1978 | HB1 | LEU | 136 | 4.193 | -7.724 | -10.365 | 1.00 | 0.27 |
| ATOM | 1979 | HB2 | LEU | 136 | 3.302 | -9.072 | -11.064 | 1.00 | 0.26 |
| ATOM | 1980 | CG | LEU | 136 | 5.213 | -8.709 | -11.980 | 1.00 | 0.26 |
| ATOM | 1981 | HG | LEU | 136 | 5.312 | -9.713 | -12.368 | 1.00 | 0.29 |
| ATOM | 1982 | CD1 | LEU | 136 | 4.624 | -7.801 | -13.063 | 1.00 | 0.29 |
| ATOM | 1983 | HD11 | LEU | 136 | 3.546 | -7.848 | -13.030 | 1.00 | 1.06 |
| ATOM | 1984 | HD12 | LEU | 136 | 4.967 | -8.126 | -14.033 | 1.00 | 1.05 |
| ATOM | 1985 | HD13 | LEU | 136 | 4.944 | -6.784 | -12.893 | 1.00 | 1.06 |
| ATOM | 1986 | CD2 | LEU | 136 | 6.592 | -8.176 | -11.578 | 1.00 | 0.32 |
| ATOM | 1987 | HD21 | LEU | 136 | 6.485 | -7.477 | -10.762 | 1.00 | 1.05 |
| ATOM | 1988 | HD22 | LEU | 136 | 7.046 | -7.677 | -12.422 | 1.00 | 1.09 |
| ATOM | 1989 | HD23 | LEU | 136 | 7.220 | -8.998 | -11.269 | 1.00 | 0.97 |
| ATOM | 1990 | C | LEU | 136 | 3.954 | -9.556 | -8.427 | 1.00 | 0.25 |
| ATOM | 1991 | O | LEU | 136 | 4.201 | -8.761 | -7.542 | 1.00 | 0.30 |
| ATOM | 1992 | N | MET | 137 | 2.924 | -10.353 | -8.357 | 1.00 | 0.28 |
| ATOM | 1993 | HN | MET | 137 | 2.744 | -10.981 | -9.087 | 1.00 | 0.31 |
| ATOM | 1994 | CA | MET | 137 | 2.016 | -10.309 | -7.177 | 1.00 | 0.33 |
| ATOM | 1995 | HA | MET | 137 | 1.768 | -9.283 | -6.959 | 1.00 | 0.38 |
| ATOM | 1996 | CB | MET | 137 | 0.734 | -11.087 | -7.494 | 1.00 | 0.42 |
| ATOM | 1997 | HB1 | MET | 137 | 0.118 | -11.136 | -6.615 | 1.00 | 0.57 |
| ATOM | 1998 | HB2 | MET | 137 | 0.995 | -12.089 | -7.803 | 1.00 | 0.50 |
| ATOM | 1999 | CG | MET | 137 | -0.035 | -10.391 | -8.625 | 1.00 | 0.58 |
| ATOM | 2000 | HG1 | MET | 137 | -0.909 | -10.975 | -8.875 | 1.00 | 1.13 |
| ATOM | 2001 | HG2 | MET | 137 | 0.601 | -10.311 | -9.494 | 1.00 | 1.22 |
| ATOM | 2002 | SD | MET | 137 | -0.551 | -8.729 | -8.108 | 1.00 | 0.83 |
| ATOM | 2003 | CE | MET | 137 | -2.048 | -9.184 | -7.194 | 1.00 | 0.39 |
| ATOM | 2004 | HE1 | MET | 137 | -2.231 | -8.450 | -6.426 | 1.00 | 1.14 |
| ATOM | 2005 | HE2 | MET | 137 | -1.927 | -10.151 | -6.741 | 1.00 | 1.07 |
| ATOM | 2006 | HE3 | MET | 137 | -2.885 | -9.212 | -7.872 | 1.00 | 1.06 |
| ATOM | 2007 | C | MET | 137 | 2.700 | -10.925 | -5.951 | 1.00 | 0.27 |
| ATOM | 2008 | O | MET | 137 | 2.050 | -11.287 | -4.990 | 1.00 | 0.28 |
| ATOM | 2009 | N | PHE | 138 | 4.000 | -11.042 | -5.964 | 1.00 | 0.25 |
| ATOM | 2010 | HN | PHE | 138 | 4.514 | -10.741 | -6.743 | 1.00 | 0.28 |
| ATOM | 2011 | CA | PHE | 138 | 4.699 | -11.628 | -4.785 | 1.00 | 0.23 |
| ATOM | 2012 | HA | PHE | 138 | 4.225 | -12.557 | -4.534 | 1.00 | 0.26 |
| ATOM | 2013 | CB | PHE | 138 | 6.167 | -11.877 | -5.152 | 1.00 | 0.25 |
| ATOM | 2014 | HB1 | PHE | 138 | 6.710 | -10.945 | -5.104 | 1.00 | 0.24 |
| ATOM | 2015 | HB2 | PHE | 138 | 6.221 | -12.270 | -6.156 | 1.00 | 0.27 |
| ATOM | 2016 | CG | PHE | 138 | 6.790 | -12.873 | -4.194 | 1.00 | 0.28 |
| ATOM | 2017 | CD1 | PHE | 138 | 6.295 | -14.184 | -4.113 | 1.00 | 0.32 |
| ATOM | 2018 | HD1 | PHE | 138 | 5.465 | -14.490 | -4.731 | 1.00 | 0.33 |
| ATOM | 2019 | CD2 | PHE | 138 | 7.871 | -12.486 | -3.392 | 1.00 | 0.30 |
| ATOM | 2020 | HD2 | PHE | 138 | 8.256 | -11.481 | -3.455 | 1.00 | 0.30 |
| ATOM | 2021 | CE1 | PHE | 138 | 6.881 | -15.100 | -3.230 | 1.00 | 0.38 |
| ATOM | 2022 | HE1 | PHE | 138 | 6.500 | -16.109 | -3.168 | 1.00 | 0.42 |
| ATOM | 2023 | CE2 | PHE | 138 | 8.455 | -13.404 | -2.511 | 1.00 | 0.36 |
| ATOM | 2024 | HE2 | PHE | 138 | 9.288 | -13.104 | -1.894 | 1.00 | 0.39 |
| ATOM | 2025 | CZ | PHE | 138 | 7.960 | -14.710 | -2.430 | 1.00 | 0.39 |
| ATOM | 2026 | HZ | PHE | 138 | 8.411 | -15.417 | -1.749 | 1.00 | 0.44 |
| ATOM | 2027 | C | PHE | 138 | 4.601 | -10.615 | -3.615 | 1.00 | 0.20 |
| ATOM | 2028 | O | PHE | 138 | 4.874 | -9.447 | -3.808 | 1.00 | 0.22 |
| ATOM | 2029 | N | PRO | 139 | 4.185 | -11.019 | -2.421 | 1.00 | 0.22 |
| ATOM | 2030 | CA | PRO | 139 | 4.044 | -10.048 | -1.291 | 1.00 | 0.25 |
| ATOM | 2031 | HA | PRO | 139 | 3.262 | -9.340 | -1.509 | 1.00 | 0.27 |
| ATOM | 2032 | CB | PRO | 139 | 3.600 | -10.936 | -0.127 | 1.00 | 0.31 |
| ATOM | 2033 | HB1 | PRO | 139 | 2.615 | -10.638 | 0.199 | 1.00 | 0.38 |
| ATOM | 2034 | HB2 | PRO | 139 | 4.299 | -10.835 | 0.691 | 1.00 | 0.42 |
| ATOM | 2035 | CG | PRO | 139 | 3.562 | -12.392 | -0.597 | 1.00 | 0.33 |
| ATOM | 2036 | HG1 | PRO | 139 | 2.588 | -12.812 | -0.396 | 1.00 | 0.41 |
| ATOM | 2037 | HG2 | PRO | 139 | 4.317 | -12.961 | -0.074 | 1.00 | 0.42 |
| ATOM | 2038 | CD | PRO | 139 | 3.834 | -12.435 | -2.102 | 1.00 | 0.27 |
| ATOM | 2039 | HD2 | PRO | 139 | 4.661 | -13.100 | -2.318 | 1.00 | 0.28 |
| ATOM | 2040 | HD1 | PRO | 139 | 2.946 | -12.732 | -2.637 | 1.00 | 0.30 |
| ATOM | 2041 | C | PRO | 139 | 5.337 | -10.305 | -0.000 | 1.00 | 0.00 |

31/75

| | | | | | | | | | |
|------|------|------|-----|-----|--------|---------|---------|------|------|
| ATOM | 2042 | O | PRO | 139 | 5.302 | -8.351 | -0.173 | 1.00 | 0.44 |
| ATOM | 2043 | N | ILE | 140 | 6.467 | -9.726 | -1.437 | 1.00 | 0.24 |
| ATOM | 2044 | HN | ILE | 140 | 6.474 | -10.500 | -2.038 | 1.00 | 0.37 |
| ATOM | 2045 | CA | ILE | 140 | 7.749 | -9.031 | -1.094 | 1.00 | 0.23 |
| ATOM | 2046 | HA | ILE | 140 | 7.572 | -8.308 | -0.312 | 1.00 | 0.24 |
| ATOM | 2047 | CB | ILE | 140 | 8.775 | -10.054 | -0.600 | 1.00 | 0.25 |
| ATOM | 2048 | HB | ILE | 140 | 8.978 | -10.770 | -1.379 | 1.00 | 0.25 |
| ATOM | 2049 | CG1 | ILE | 140 | 8.207 | -10.768 | 0.632 | 1.00 | 0.29 |
| ATOM | 2050 | HG11 | ILE | 140 | 7.246 | -11.196 | 0.384 | 1.00 | 0.32 |
| ATOM | 2051 | HG12 | ILE | 140 | 8.084 | -10.055 | 1.434 | 1.00 | 0.33 |
| ATOM | 2052 | CG2 | ILE | 140 | 10.070 | -9.332 | -0.214 | 1.00 | 0.26 |
| ATOM | 2053 | HG21 | ILE | 140 | 9.850 | -8.567 | 0.517 | 1.00 | 1.04 |
| ATOM | 2054 | HG22 | ILE | 140 | 10.505 | -8.876 | -1.090 | 1.00 | 1.06 |
| ATOM | 2055 | HG23 | ILE | 140 | 10.768 | -10.040 | 0.207 | 1.00 | 1.04 |
| ATOM | 2056 | CD1 | ILE | 140 | 9.156 | -11.883 | 1.082 | 1.00 | 0.30 |
| ATOM | 2057 | HD11 | ILE | 140 | 9.716 | -12.250 | 0.236 | 1.00 | 1.08 |
| ATOM | 2058 | HD12 | ILE | 140 | 8.582 | -12.691 | 1.511 | 1.00 | 0.98 |
| ATOM | 2059 | HD13 | ILE | 140 | 9.838 | -11.495 | 1.824 | 1.00 | 1.08 |
| ATOM | 2060 | C | ILE | 140 | 8.284 | -8.301 | -2.329 | 1.00 | 0.22 |
| ATOM | 2061 | O | ILE | 140 | 8.265 | -8.817 | -3.429 | 1.00 | 0.22 |
| ATOM | 2062 | N | TYR | 141 | 8.745 | -7.092 | -2.150 | 1.00 | 0.21 |
| ATOM | 2063 | HN | TYR | 141 | 8.736 | -6.696 | -1.254 | 1.00 | 0.22 |
| ATOM | 2064 | CA | TYR | 141 | 9.265 | -6.303 | -3.304 | 1.00 | 0.21 |
| ATOM | 2065 | HA | TYR | 141 | 8.560 | -6.348 | -4.120 | 1.00 | 0.20 |
| ATOM | 2066 | CB | TYR | 141 | 9.444 | -4.847 | -2.865 | 1.00 | 0.21 |
| ATOM | 2067 | HB1 | TYR | 141 | 10.050 | -4.810 | -1.972 | 1.00 | 0.22 |
| ATOM | 2068 | HB2 | TYR | 141 | 8.476 | -4.413 | -2.661 | 1.00 | 0.22 |
| ATOM | 2069 | CG | TYR | 141 | 10.122 | -4.066 | -3.962 | 1.00 | 0.23 |
| ATOM | 2070 | CD1 | TYR | 141 | 11.515 | -4.104 | -4.089 | 1.00 | 0.25 |
| ATOM | 2071 | HD1 | TYR | 141 | 12.104 | -4.697 | -3.404 | 1.00 | 0.26 |
| ATOM | 2072 | CD2 | TYR | 141 | 9.359 | -3.298 | -4.848 | 1.00 | 0.24 |
| ATOM | 2073 | HD2 | TYR | 141 | 8.284 | -3.268 | -4.750 | 1.00 | 0.25 |
| ATOM | 2074 | CE1 | TYR | 141 | 12.146 | -3.376 | -5.103 | 1.00 | 0.28 |
| ATOM | 2075 | HE1 | TYR | 141 | 13.221 | -3.405 | -5.201 | 1.00 | 0.32 |
| ATOM | 2076 | CE2 | TYR | 141 | 9.989 | -2.569 | -5.862 | 1.00 | 0.27 |
| ATOM | 2077 | HE2 | TYR | 141 | 9.401 | -1.975 | -6.544 | 1.00 | 0.30 |
| ATOM | 2078 | CZ | TYR | 141 | 11.383 | -2.608 | -5.990 | 1.00 | 0.29 |
| ATOM | 2079 | OH | TYR | 141 | 12.005 | -1.892 | -6.991 | 1.00 | 0.33 |
| ATOM | 2080 | HH | TYR | 141 | 12.781 | -2.385 | -7.269 | 1.00 | 0.90 |
| ATOM | 2081 | C | TYR | 141 | 10.615 | -6.864 | -3.761 | 1.00 | 0.22 |
| ATOM | 2082 | O | TYR | 141 | 11.522 | -7.050 | -2.973 | 1.00 | 0.23 |
| ATOM | 2083 | N | THR | 142 | 10.750 | -7.130 | -5.035 | 1.00 | 0.22 |
| ATOM | 2084 | HN | THR | 142 | 10.002 | -6.968 | -5.648 | 1.00 | 0.22 |
| ATOM | 2085 | CA | THR | 142 | 12.035 | -7.675 | -5.563 | 1.00 | 0.24 |
| ATOM | 2086 | HA | THR | 142 | 12.835 | -7.447 | -4.874 | 1.00 | 0.25 |
| ATOM | 2087 | CB | THR | 142 | 11.917 | -9.193 | -5.723 | 1.00 | 0.25 |
| ATOM | 2088 | HB | THR | 142 | 11.645 | -9.635 | -4.777 | 1.00 | 0.26 |
| ATOM | 2089 | OG1 | THR | 142 | 13.165 | -9.720 | -6.152 | 1.00 | 0.29 |
| ATOM | 2090 | HG1 | THR | 142 | 13.274 | -9.505 | -7.081 | 1.00 | 0.97 |
| ATOM | 2091 | CG2 | THR | 142 | 10.840 | -9.517 | -6.760 | 1.00 | 0.25 |
| ATOM | 2092 | HG21 | THR | 142 | 10.577 | -10.562 | -6.691 | 1.00 | 1.04 |
| ATOM | 2093 | HG22 | THR | 142 | 11.217 | -9.304 | -7.749 | 1.00 | 1.05 |
| ATOM | 2094 | HG23 | THR | 142 | 9.965 | -8.913 | -6.570 | 1.00 | 1.06 |
| ATOM | 2095 | C | THR | 142 | 12.339 | -7.040 | -6.924 | 1.00 | 0.23 |
| ATOM | 2096 | O | THR | 142 | 11.454 | -6.810 | -7.724 | 1.00 | 0.23 |
| ATOM | 2097 | N | TYR | 143 | 13.586 | -6.758 | -7.195 | 1.00 | 0.25 |
| ATOM | 2098 | HN | TYR | 143 | 14.285 | -6.955 | -6.538 | 1.00 | 0.27 |
| ATOM | 2099 | CA | TYR | 143 | 13.948 | -6.144 | -8.506 | 1.00 | 0.26 |
| ATOM | 2100 | HA | TYR | 143 | 13.174 | -5.452 | -8.804 | 1.00 | 0.25 |
| ATOM | 2101 | CB | TYR | 143 | 15.277 | -5.395 | -8.370 | 1.00 | 0.29 |
| ATOM | 2102 | HB1 | TYR | 143 | 16.072 | -6.104 | -8.190 | 1.00 | 0.33 |
| ATOM | 2103 | HB2 | TYR | 143 | 15.217 | -4.704 | -7.542 | 1.00 | 0.30 |
| ATOM | 2104 | CG | TYR | 143 | 15.563 | -4.633 | -9.642 | 1.00 | 0.27 |
| ATOM | 2105 | CD1 | TYR | 143 | 14.931 | -3.406 | -9.880 | 1.00 | 0.25 |
| ATOM | 2106 | HD1 | TYR | 143 | 14.234 | -3.008 | -9.156 | 1.00 | 0.26 |
| ATOM | 2107 | CD2 | TYR | 143 | 16.466 | -5.148 | -10.581 | 1.00 | 0.31 |
| ATOM | 2108 | HD2 | TYR | 143 | 16.954 | -6.094 | -10.398 | 1.00 | 0.35 |
| ATOM | 2109 | CE1 | TYR | 143 | 15.201 | -2.695 | -11.055 | 1.00 | 0.26 |
| ATOM | 2110 | HE1 | TYR | 143 | 14.713 | -1.749 | -11.238 | 1.00 | 0.28 |
| ATOM | 2111 | CE2 | TYR | 143 | 16.735 | -4.436 | -11.756 | 1.00 | 0.31 |
| ATOM | 2112 | HE2 | TYR | 143 | 17.432 | -4.833 | -12.480 | 1.00 | 0.36 |
| ATOM | 2113 | CZ | TYR | 143 | 16.103 | -3.210 | -11.994 | 1.00 | 0.28 |
| ATOM | 2114 | OH | TYR | 143 | 16.369 | -2.509 | -13.152 | 1.00 | 0.30 |
| ATOM | 2115 | HH | TYR | 143 | 17.068 | -2.969 | -13.624 | 1.00 | 0.95 |
| ATOM | 2116 | C | TYR | 143 | 14.080 | -7.244 | -9.563 | 1.00 | 0.27 |
| ATOM | 2117 | O | TYR | 143 | 14.552 | -8.328 | -9.283 | 1.00 | 0.31 |
| ATOM | 2118 | N | THR | 144 | 13.660 | -6.876 | -8.773 | 1.00 | 0.22 |

32/75

| | | | | | | | | | |
|------|------|------|-----|-----|--------|---------|---------|------|------|
| ATOM | 2119 | HN | THR | 144 | 13.277 | -6.096 | -10.972 | 1.00 | 0.32 |
| ATOM | 2120 | CA | THR | 144 | 13.753 | -8.008 | -11.847 | 1.00 | 0.32 |
| ATOM | 2121 | HA | THR | 144 | 14.479 | -8.758 | -11.573 | 1.00 | 0.35 |
| ATOM | 2122 | CB | THR | 144 | 12.385 | -8.666 | -12.031 | 1.00 | 0.37 |
| ATOM | 2123 | HB | THR | 144 | 11.922 | -8.814 | -11.067 | 1.00 | 0.84 |
| ATOM | 2124 | OG1 | THR | 144 | 12.549 | -9.918 | -12.683 | 1.00 | 1.00 |
| ATOM | 2125 | HG1 | THR | 144 | 13.280 | -9.836 | -13.301 | 1.00 | 1.42 |
| ATOM | 2126 | CG2 | THR | 144 | 11.499 | -7.757 | -12.882 | 1.00 | 0.82 |
| ATOM | 2127 | HG21 | THR | 144 | 10.461 | -7.991 | -12.699 | 1.00 | 1.51 |
| ATOM | 2128 | HG22 | THR | 144 | 11.724 | -7.911 | -13.927 | 1.00 | 1.24 |
| ATOM | 2129 | HG23 | THR | 144 | 11.687 | -6.726 | -12.622 | 1.00 | 1.49 |
| ATOM | 2130 | C | THR | 144 | 14.169 | -7.351 | -13.165 | 1.00 | 0.34 |
| ATOM | 2131 | O | THR | 144 | 13.922 | -6.183 | -13.392 | 1.00 | 0.32 |
| ATOM | 2132 | N | GLY | 145 | 14.789 | -8.094 | -14.043 | 1.00 | 0.43 |
| ATOM | 2133 | HN | GLY | 145 | 14.971 | -9.037 | -13.846 | 1.00 | 0.49 |
| ATOM | 2134 | CA | GLY | 145 | 15.205 | -7.510 | -15.350 | 1.00 | 0.49 |
| ATOM | 2135 | HA1 | GLY | 145 | 15.842 | -8.207 | -15.872 | 1.00 | 0.57 |
| ATOM | 2136 | HA2 | GLY | 145 | 15.742 | -6.587 | -15.178 | 1.00 | 0.50 |
| ATOM | 2137 | C | GLY | 145 | 13.957 | -7.233 | -16.191 | 1.00 | 0.47 |
| ATOM | 2138 | O | GLY | 145 | 13.331 | -8.138 | -16.706 | 1.00 | 0.53 |
| ATOM | 2139 | N | LYS | 146 | 13.583 | -5.990 | -16.322 | 1.00 | 0.46 |
| ATOM | 2140 | HN | LYS | 146 | 14.097 | -5.277 | -15.889 | 1.00 | 0.48 |
| ATOM | 2141 | CA | LYS | 146 | 12.367 | -5.653 | -17.116 | 1.00 | 0.49 |
| ATOM | 2142 | HA | LYS | 146 | 11.578 | -6.350 | -16.876 | 1.00 | 0.51 |
| ATOM | 2143 | CB | LYS | 146 | 11.911 | -4.235 | -16.764 | 1.00 | 0.52 |
| ATOM | 2144 | HB1 | LYS | 146 | 10.973 | -4.032 | -17.254 | 1.00 | 0.58 |
| ATOM | 2145 | HB2 | LYS | 146 | 12.657 | -3.533 | -17.103 | 1.00 | 0.57 |
| ATOM | 2146 | CG | LYS | 146 | 11.744 | -4.128 | -15.238 | 1.00 | 0.55 |
| ATOM | 2147 | HG1 | LYS | 146 | 12.690 | -3.853 | -14.798 | 1.00 | 0.83 |
| ATOM | 2148 | HG2 | LYS | 146 | 11.442 | -5.089 | -14.849 | 1.00 | 1.14 |
| ATOM | 2149 | CD | LYS | 146 | 10.684 | -3.077 | -14.854 | 1.00 | 1.23 |
| ATOM | 2150 | HD1 | LYS | 146 | 10.308 | -3.309 | -13.871 | 1.00 | 1.78 |
| ATOM | 2151 | HD2 | LYS | 146 | 9.865 | -3.098 | -15.556 | 1.00 | 1.79 |
| ATOM | 2152 | CE | LYS | 146 | 11.298 | -1.671 | -14.828 | 1.00 | 2.01 |
| ATOM | 2153 | HE1 | LYS | 146 | 11.615 | -1.439 | -13.822 | 1.00 | 2.47 |
| ATOM | 2154 | HE2 | LYS | 146 | 10.556 | -0.952 | -15.143 | 1.00 | 2.39 |
| ATOM | 2155 | NZ | LYS | 146 | 12.468 | -1.601 | -15.745 | 1.00 | 2.91 |
| ATOM | 2156 | HZ1 | LYS | 146 | 12.847 | -0.633 | -15.750 | 1.00 | 3.39 |
| ATOM | 2157 | HZ2 | LYS | 146 | 12.170 | -1.861 | -16.707 | 1.00 | 3.28 |
| ATOM | 2158 | HZ3 | LYS | 146 | 13.205 | -2.257 | -15.420 | 1.00 | 3.27 |
| ATOM | 2159 | C | LYS | 146 | 12.677 | -5.732 | -18.613 | 1.00 | 0.59 |
| ATOM | 2160 | O | LYS | 146 | 11.845 | -5.426 | -19.444 | 1.00 | 1.16 |
| ATOM | 2161 | N | SER | 147 | 13.868 | -6.131 | -18.967 | 1.00 | 0.78 |
| ATOM | 2162 | HN | SER | 147 | 14.530 | -6.366 | -18.283 | 1.00 | 1.26 |
| ATOM | 2163 | CA | SER | 147 | 14.226 | -6.214 | -20.413 | 1.00 | 0.87 |
| ATOM | 2164 | HA | SER | 147 | 14.141 | -5.234 | -20.859 | 1.00 | 1.03 |
| ATOM | 2165 | CB | SER | 147 | 15.667 | -6.709 | -20.554 | 1.00 | 0.95 |
| ATOM | 2166 | HB1 | SER | 147 | 15.798 | -7.158 | -21.530 | 1.00 | 1.42 |
| ATOM | 2167 | HB2 | SER | 147 | 15.871 | -7.445 | -19.794 | 1.00 | 1.34 |
| ATOM | 2168 | OG | SER | 147 | 16.561 | -5.616 | -20.395 | 1.00 | 1.71 |
| ATOM | 2169 | HG | SER | 147 | 17.097 | -5.555 | -21.190 | 1.00 | 2.16 |
| ATOM | 2170 | C | SER | 147 | 13.288 | -7.185 | -21.138 | 1.00 | 0.79 |
| ATOM | 2171 | O | SER | 147 | 12.747 | -6.865 | -22.178 | 1.00 | 1.40 |
| ATOM | 2172 | N | HIS | 148 | 13.098 | -8.366 | -20.605 | 1.00 | 0.66 |
| ATOM | 2173 | HN | HIS | 148 | 13.551 | -8.602 | -19.768 | 1.00 | 1.10 |
| ATOM | 2174 | CA | HIS | 148 | 12.199 | -9.360 | -21.272 | 1.00 | 0.65 |
| ATOM | 2175 | HA | HIS | 148 | 11.629 | -8.874 | -22.048 | 1.00 | 0.74 |
| ATOM | 2176 | CB | HIS | 148 | 13.041 | -10.479 | -21.887 | 1.00 | 0.79 |
| ATOM | 2177 | HB1 | HIS | 148 | 12.401 | -11.312 | -22.138 | 1.00 | 1.14 |
| ATOM | 2178 | HB2 | HIS | 148 | 13.786 | -10.801 | -21.174 | 1.00 | 1.30 |
| ATOM | 2179 | CG | HIS | 148 | 13.723 | -9.980 | -23.130 | 1.00 | 1.66 |
| ATOM | 2180 | ND1 | HIS | 148 | 13.104 | -9.116 | -24.019 | 1.00 | 2.52 |
| ATOM | 2181 | HD1 | HIS | 148 | 12.200 | -8.747 | -23.934 | 1.00 | 2.81 |
| ATOM | 2182 | CD2 | HIS | 148 | 14.969 | -10.226 | -23.652 | 1.00 | 2.62 |
| ATOM | 2183 | HD2 | HIS | 148 | 15.715 | -10.867 | -23.206 | 1.00 | 3.00 |
| ATOM | 2184 | CE1 | HIS | 148 | 13.970 | -8.875 | -25.020 | 1.00 | 3.46 |
| ATOM | 2185 | HE1 | HIS | 148 | 13.759 | -8.233 | -25.863 | 1.00 | 4.33 |
| ATOM | 2186 | NE2 | HIS | 148 | 15.123 | -9.528 | -24.846 | 1.00 | 3.55 |
| ATOM | 2187 | C | HIS | 148 | 11.238 | -9.971 | -20.249 | 1.00 | 0.55 |
| ATOM | 2188 | O | HIS | 148 | 10.743 | -11.064 | -20.435 | 1.00 | 0.60 |
| ATOM | 2189 | N | PHE | 149 | 10.978 | -9.293 | -19.167 | 1.00 | 0.57 |
| ATOM | 2190 | HN | PHE | 149 | 11.392 | -8.417 | -19.021 | 1.00 | 0.73 |
| ATOM | 2191 | CA | PHE | 149 | 10.060 | -9.871 | -18.145 | 1.00 | 0.48 |
| ATOM | 2192 | HA | PHE | 149 | 10.416 | -10.849 | -17.857 | 1.00 | 0.51 |
| ATOM | 2193 | CB | PHE | 149 | 10.022 | -8.967 | -16.911 | 1.00 | 0.44 |
| ATOM | 2194 | HB1 | PHE | 149 | 9.603 | -8.008 | -17.177 | 1.00 | 0.44 |
| ATOM | 2195 | HB2 | PHE | 149 | 11.023 | -8.831 | -16.530 | 1.00 | 0.49 |

33/75

| | | | | | | | | | |
|------|------|------|-----|-----|--------|---------|---------|------|------|
| ATOM | 2196 | CG | PHE | 149 | 9.161 | -9.615 | -15.851 | 1.00 | 0.40 |
| ATOM | 2197 | CD1 | PHE | 149 | 7.766 | -9.507 | -15.919 | 1.00 | 0.36 |
| ATOM | 2198 | HD1 | PHE | 149 | 7.305 | -8.956 | -16.726 | 1.00 | 0.38 |
| ATOM | 2199 | CD2 | PHE | 149 | 9.757 | -10.328 | -14.804 | 1.00 | 0.42 |
| ATOM | 2200 | HD2 | PHE | 149 | 10.832 | -10.412 | -14.750 | 1.00 | 0.48 |
| ATOM | 2201 | CE1 | PHE | 149 | 6.969 | -10.112 | -14.941 | 1.00 | 0.35 |
| ATOM | 2202 | HE1 | PHE | 149 | 5.894 | -10.031 | -14.996 | 1.00 | 0.37 |
| ATOM | 2203 | CE2 | PHE | 149 | 8.958 | -10.932 | -13.825 | 1.00 | 0.40 |
| ATOM | 2204 | HE2 | PHE | 149 | 9.417 | -11.482 | -13.016 | 1.00 | 0.45 |
| ATOM | 2205 | CZ | PHE | 149 | 7.564 | -10.825 | -13.894 | 1.00 | 0.37 |
| ATOM | 2206 | HZ | PHE | 149 | 6.948 | -11.291 | -13.140 | 1.00 | 0.38 |
| ATOM | 2207 | C | PHE | 149 | 8.641 | -9.993 | -18.706 | 1.00 | 0.43 |
| ATOM | 2208 | O | PHE | 149 | 8.080 | -9.044 | -19.217 | 1.00 | 0.45 |
| ATOM | 2209 | N | MET | 150 | 8.050 | -11.153 | -18.575 | 1.00 | 0.43 |
| ATOM | 2210 | HN | MET | 150 | 8.523 | -11.888 | -18.133 | 1.00 | 0.50 |
| ATOM | 2211 | CA | MET | 150 | 6.651 | -11.357 | -19.051 | 1.00 | 0.39 |
| ATOM | 2212 | HA | MET | 150 | 6.189 | -10.400 | -19.245 | 1.00 | 0.38 |
| ATOM | 2213 | CB | MET | 150 | 6.632 | -12.207 | -20.328 | 1.00 | 0.44 |
| ATOM | 2214 | HB1 | MET | 150 | 5.610 | -12.374 | -20.632 | 1.00 | 0.45 |
| ATOM | 2215 | HB2 | MET | 150 | 7.109 | -13.157 | -20.134 | 1.00 | 0.47 |
| ATOM | 2216 | CG | MET | 150 | 7.381 | -11.477 | -21.446 | 1.00 | 0.50 |
| ATOM | 2217 | HG1 | MET | 150 | 8.401 | -11.831 | -21.485 | 1.00 | 0.98 |
| ATOM | 2218 | HG2 | MET | 150 | 7.376 | -10.415 | -21.253 | 1.00 | 0.86 |
| ATOM | 2219 | SD | MET | 150 | 6.571 | -11.806 | -23.033 | 1.00 | 1.32 |
| ATOM | 2220 | CE | MET | 150 | 7.378 | -13.384 | -23.393 | 1.00 | 2.23 |
| ATOM | 2221 | HE1 | MET | 150 | 7.326 | -14.022 | -22.521 | 1.00 | 2.66 |
| ATOM | 2222 | HE2 | MET | 150 | 8.411 | -13.211 | -23.647 | 1.00 | 2.74 |
| ATOM | 2223 | HE3 | MET | 150 | 6.879 | -13.861 | -24.225 | 1.00 | 2.74 |
| ATOM | 2224 | C | MET | 150 | 5.877 | -12.071 | -17.943 | 1.00 | 0.32 |
| ATOM | 2225 | O | MET | 150 | 6.435 | -12.837 | -17.183 | 1.00 | 0.32 |
| ATOM | 2226 | N | LEU | 151 | 4.605 | -11.819 | -17.827 | 1.00 | 0.28 |
| ATOM | 2227 | HN | LEU | 151 | 4.169 | -11.188 | -18.437 | 1.00 | 0.30 |
| ATOM | 2228 | CA | LEU | 151 | 3.821 | -12.478 | -16.746 | 1.00 | 0.24 |
| ATOM | 2229 | HA | LEU | 151 | 4.120 | -12.064 | -15.803 | 1.00 | 0.24 |
| ATOM | 2230 | CB | LEU | 151 | 2.327 | -12.212 | -16.966 | 1.00 | 0.24 |
| ATOM | 2231 | HB1 | LEU | 151 | 1.765 | -12.626 | -16.145 | 1.00 | 0.25 |
| ATOM | 2232 | HB2 | LEU | 151 | 2.012 | -12.680 | -17.887 | 1.00 | 0.28 |
| ATOM | 2233 | CG | LEU | 151 | 2.061 | -10.703 | -17.047 | 1.00 | 0.28 |
| ATOM | 2234 | HG | LEU | 151 | 2.900 | -10.208 | -17.512 | 1.00 | 0.52 |
| ATOM | 2235 | CD1 | LEU | 151 | 0.804 | -10.457 | -17.881 | 1.00 | 0.35 |
| ATOM | 2236 | HD11 | LEU | 151 | 0.506 | -9.424 | -17.788 | 1.00 | 1.07 |
| ATOM | 2237 | HD12 | LEU | 151 | 0.007 | -11.095 | -17.526 | 1.00 | 1.02 |
| ATOM | 2238 | HD13 | LEU | 151 | 1.009 | -10.682 | -18.917 | 1.00 | 1.17 |
| ATOM | 2239 | CD2 | LEU | 151 | 1.848 | -10.140 | -15.638 | 1.00 | 0.46 |
| ATOM | 2240 | HD21 | LEU | 151 | 2.078 | -9.084 | -15.635 | 1.00 | 1.14 |
| ATOM | 2241 | HD22 | LEU | 151 | 2.495 | -10.650 | -14.941 | 1.00 | 1.16 |
| ATOM | 2242 | HD23 | LEU | 151 | 0.820 | -10.284 | -15.345 | 1.00 | 1.11 |
| ATOM | 2243 | C | LEU | 151 | 4.076 | -14.004 | -16.794 | 1.00 | 0.24 |
| ATOM | 2244 | O | LEU | 151 | 3.879 | -14.613 | -17.826 | 1.00 | 0.28 |
| ATOM | 2245 | N | PRO | 152 | 4.504 | -14.641 | -15.711 | 1.00 | 0.22 |
| ATOM | 2246 | CA | PRO | 152 | 4.748 | -16.112 | -15.751 | 1.00 | 0.23 |
| ATOM | 2247 | HA | PRO | 152 | 5.480 | -16.354 | -16.503 | 1.00 | 0.24 |
| ATOM | 2248 | CB | PRO | 152 | 5.323 | -16.404 | -14.364 | 1.00 | 0.24 |
| ATOM | 2249 | HB1 | PRO | 152 | 6.361 | -16.686 | -14.453 | 1.00 | 0.29 |
| ATOM | 2250 | HB2 | PRO | 152 | 4.766 | -17.208 | -13.903 | 1.00 | 0.26 |
| ATOM | 2251 | CG | PRO | 152 | 5.209 | -15.141 | -13.507 | 1.00 | 0.32 |
| ATOM | 2252 | HG1 | PRO | 152 | 6.166 | -14.917 | -13.061 | 1.00 | 0.44 |
| ATOM | 2253 | HG2 | PRO | 152 | 4.473 | -15.295 | -12.730 | 1.00 | 0.41 |
| ATOM | 2254 | CD | PRO | 152 | 4.778 | -13.976 | -14.402 | 1.00 | 0.25 |
| ATOM | 2255 | HD2 | PRO | 152 | 3.886 | -13.507 | -14.008 | 1.00 | 0.25 |
| ATOM | 2256 | HD1 | PRO | 152 | 5.581 | -13.263 | -14.503 | 1.00 | 0.27 |
| ATOM | 2257 | C | PRO | 152 | 3.462 | -16.915 | -15.974 | 1.00 | 0.21 |
| ATOM | 2258 | O | PRO | 152 | 2.378 | -16.371 | -16.038 | 1.00 | 0.20 |
| ATOM | 2259 | N | ASP | 153 | 3.582 | -18.209 | -16.090 | 1.00 | 0.23 |
| ATOM | 2260 | HN | ASP | 153 | 4.468 | -18.622 | -16.031 | 1.00 | 0.25 |
| ATOM | 2261 | CA | ASP | 153 | 2.380 | -19.063 | -16.304 | 1.00 | 0.23 |
| ATOM | 2262 | HA | ASP | 153 | 1.890 | -18.772 | -17.221 | 1.00 | 0.23 |
| ATOM | 2263 | CB | ASP | 153 | 2.813 | -20.526 | -16.401 | 1.00 | 0.25 |
| ATOM | 2264 | HB1 | ASP | 153 | 1.943 | -21.163 | -16.363 | 1.00 | 0.26 |
| ATOM | 2265 | HB2 | ASP | 153 | 3.470 | -20.762 | -15.576 | 1.00 | 0.26 |
| ATOM | 2266 | CG | ASP | 153 | 3.550 | -20.752 | -17.722 | 1.00 | 0.27 |
| ATOM | 2267 | OD1 | ASP | 153 | 4.768 | -20.687 | -17.717 | 1.00 | 1.08 |
| ATOM | 2268 | OD2 | ASP | 153 | 2.884 | -20.994 | -18.715 | 1.00 | 1.14 |
| ATOM | 2269 | C | ASP | 153 | 1.409 | -18.899 | -15.133 | 1.00 | 0.21 |
| ATOM | 2270 | O | ASP | 153 | 0.208 | -18.858 | -15.310 | 1.00 | 0.21 |
| ATOM | 2271 | N | ASP | 154 | 1.919 | -18.820 | -13.935 | 1.00 | 0.21 |
| ATOM | 2272 | HN | ASP | 154 | 2.881 | -18.866 | -13.811 | 1.00 | 0.22 |

34/75

| | | | | | | | | | |
|------|------|------|-----|-----|--------|---------|---------|------|------|
| ATOM | 2273 | CA | ASP | 154 | 1.025 | -18.678 | -12.752 | 1.00 | 0.21 |
| ATOM | 2274 | HA | ASP | 154 | 0.431 | -19.572 | -12.641 | 1.00 | 0.22 |
| ATOM | 2275 | CB | ASP | 154 | 1.880 | -18.474 | -11.496 | 1.00 | 0.23 |
| ATOM | 2276 | HB1 | ASP | 154 | 2.466 | -17.572 | -11.602 | 1.00 | 0.22 |
| ATOM | 2277 | HB2 | ASP | 154 | 2.541 | -19.319 | -11.370 | 1.00 | 0.25 |
| ATOM | 2278 | CG | ASP | 154 | 0.975 | -18.347 | -10.267 | 1.00 | 0.25 |
| ATOM | 2279 | OD1 | ASP | 154 | 1.276 | -18.982 | -9.269 | 1.00 | 1.13 |
| ATOM | 2280 | OD2 | ASP | 154 | 0.004 | -17.613 | -10.340 | 1.00 | 1.07 |
| ATOM | 2281 | C | ASP | 154 | 0.102 | -17.473 | -12.943 | 1.00 | 0.19 |
| ATOM | 2282 | O | ASP | 154 | -1.095 | -17.564 | -12.759 | 1.00 | 0.19 |
| ATOM | 2283 | N | ASP | 155 | 0.645 | -16.345 | -13.303 | 1.00 | 0.19 |
| ATOM | 2284 | HN | ASP | 155 | 1.613 | -16.288 | -13.443 | 1.00 | 0.21 |
| ATOM | 2285 | CA | ASP | 155 | -0.210 | -15.140 | -13.496 | 1.00 | 0.19 |
| ATOM | 2286 | HA | ASP | 155 | -0.843 | -15.011 | -12.631 | 1.00 | 0.20 |
| ATOM | 2287 | CB | ASP | 155 | 0.683 | -13.909 | -13.653 | 1.00 | 0.21 |
| ATOM | 2288 | HB1 | ASP | 155 | 0.087 | -13.067 | -13.969 | 1.00 | 0.22 |
| ATOM | 2289 | HB2 | ASP | 155 | 1.443 | -14.113 | -14.393 | 1.00 | 0.22 |
| ATOM | 2290 | CG | ASP | 155 | 1.351 | -13.588 | -12.315 | 1.00 | 0.24 |
| ATOM | 2291 | OD1 | ASP | 155 | 2.355 | -12.896 | -12.327 | 1.00 | 1.07 |
| ATOM | 2292 | OD2 | ASP | 155 | 0.845 | -14.038 | -11.300 | 1.00 | 1.14 |
| ATOM | 2293 | C | ASP | 155 | -1.087 | -15.300 | -14.744 | 1.00 | 0.19 |
| ATOM | 2294 | O | ASP | 155 | -2.240 | -14.918 | -14.750 | 1.00 | 0.19 |
| ATOM | 2295 | N | VAL | 156 | -0.555 | -15.850 | -15.802 | 1.00 | 0.19 |
| ATOM | 2296 | HN | VAL | 156 | 0.379 | -16.147 | -15.787 | 1.00 | 0.19 |
| ATOM | 2297 | CA | VAL | 156 | -1.372 | -16.013 | -17.041 | 1.00 | 0.21 |
| ATOM | 2298 | HA | VAL | 156 | -1.726 | -15.044 | -17.362 | 1.00 | 0.22 |
| ATOM | 2299 | CB | VAL | 156 | -0.519 | -16.630 | -18.148 | 1.00 | 0.23 |
| ATOM | 2300 | HB | VAL | 156 | -0.034 | -17.521 | -17.776 | 1.00 | 0.23 |
| ATOM | 2301 | CG1 | VAL | 156 | -1.416 | -16.995 | -19.333 | 1.00 | 0.27 |
| ATOM | 2302 | HG11 | VAL | 156 | -2.273 | -16.338 | -19.348 | 1.00 | 1.00 |
| ATOM | 2303 | HG12 | VAL | 156 | -1.747 | -18.018 | -19.235 | 1.00 | 1.05 |
| ATOM | 2304 | HG13 | VAL | 156 | -0.861 | -16.882 | -20.253 | 1.00 | 1.05 |
| ATOM | 2305 | CG2 | VAL | 156 | 0.535 | -15.618 | -18.600 | 1.00 | 0.26 |
| ATOM | 2306 | HG21 | VAL | 156 | 0.990 | -15.162 | -17.733 | 1.00 | 1.07 |
| ATOM | 2307 | HG22 | VAL | 156 | 0.067 | -14.856 | -19.204 | 1.00 | 1.05 |
| ATOM | 2308 | HG23 | VAL | 156 | 1.293 | -16.123 | -19.180 | 1.00 | 1.00 |
| ATOM | 2309 | C | VAL | 156 | -2.574 | -16.919 | -16.754 | 1.00 | 0.20 |
| ATOM | 2310 | O | VAL | 156 | -3.694 | -16.615 | -17.107 | 1.00 | 0.21 |
| ATOM | 2311 | N | GLN | 157 | -2.356 | -18.035 | -16.124 | 1.00 | 0.20 |
| ATOM | 2312 | HN | GLN | 157 | -1.447 | -18.277 | -15.847 | 1.00 | 0.20 |
| ATOM | 2313 | CA | GLN | 157 | -3.498 | -18.941 | -15.824 | 1.00 | 0.22 |
| ATOM | 2314 | HA | GLN | 157 | -3.987 | -19.214 | -16.747 | 1.00 | 0.24 |
| ATOM | 2315 | CB | GLN | 157 | -2.995 | -20.204 | -15.117 | 1.00 | 0.24 |
| ATOM | 2316 | HB1 | GLN | 157 | -3.838 | -20.774 | -14.756 | 1.00 | 0.26 |
| ATOM | 2317 | HB2 | GLN | 157 | -2.368 | -19.922 | -14.282 | 1.00 | 0.23 |
| ATOM | 2318 | CG | GLN | 157 | -2.184 | -21.064 | -16.095 | 1.00 | 0.25 |
| ATOM | 2319 | HG1 | GLN | 157 | -1.174 | -20.686 | -16.152 | 1.00 | 0.94 |
| ATOM | 2320 | HG2 | GLN | 157 | -2.636 | -21.032 | -17.074 | 1.00 | 0.87 |
| ATOM | 2321 | CD | GLN | 157 | -2.152 | -22.510 | -15.598 | 1.00 | 1.19 |
| ATOM | 2322 | OE1 | GLN | 157 | -2.594 | -22.799 | -14.504 | 1.00 | 1.89 |
| ATOM | 2323 | NE2 | GLN | 157 | -1.646 | -23.437 | -16.364 | 1.00 | 1.96 |
| ATOM | 2324 | HE21 | GLN | 157 | -1.291 | -23.203 | -17.247 | 1.00 | 2.18 |
| ATOM | 2325 | HE22 | GLN | 157 | -1.624 | -24.368 | -16.058 | 1.00 | 2.65 |
| ATOM | 2326 | C | GLN | 157 | -4.505 | -18.214 | -14.925 | 1.00 | 0.22 |
| ATOM | 2327 | O | GLN | 157 | -5.702 | -18.356 | -15.077 | 1.00 | 0.24 |
| ATOM | 2328 | N | GLY | 158 | -4.027 | -17.456 | -13.974 | 1.00 | 0.21 |
| ATOM | 2329 | HN | GLY | 158 | -3.057 | -17.370 | -13.859 | 1.00 | 0.20 |
| ATOM | 2330 | CA | GLY | 158 | -4.952 | -16.741 | -13.045 | 1.00 | 0.22 |
| ATOM | 2331 | HA1 | GLY | 158 | -4.380 | -16.319 | -12.232 | 1.00 | 0.22 |
| ATOM | 2332 | HA2 | GLY | 158 | -5.667 | -17.446 | -12.646 | 1.00 | 0.25 |
| ATOM | 2333 | C | GLY | 158 | -5.704 | -15.615 | -13.766 | 1.00 | 0.20 |
| ATOM | 2334 | O | GLY | 158 | -6.918 | -15.552 | -13.730 | 1.00 | 0.21 |
| ATOM | 2335 | N | ILE | 159 | -5.007 | -14.713 | -14.405 | 1.00 | 0.18 |
| ATOM | 2336 | HN | ILE | 159 | -4.028 | -14.763 | -14.418 | 1.00 | 0.18 |
| ATOM | 2337 | CA | ILE | 159 | -5.713 | -13.593 | -15.097 | 1.00 | 0.19 |
| ATOM | 2338 | HA | ILE | 159 | -6.301 | -13.054 | -14.375 | 1.00 | 0.20 |
| ATOM | 2339 | CB | ILE | 159 | -4.679 | -12.648 | -15.735 | 1.00 | 0.19 |
| ATOM | 2340 | HB | ILE | 159 | -3.950 | -12.367 | -14.988 | 1.00 | 0.20 |
| ATOM | 2341 | CG1 | ILE | 159 | -5.355 | -11.384 | -16.284 | 1.00 | 0.24 |
| ATOM | 2342 | HG11 | ILE | 159 | -6.308 | -11.645 | -16.717 | 1.00 | 0.26 |
| ATOM | 2343 | HG12 | ILE | 159 | -4.725 | -10.952 | -17.045 | 1.00 | 0.28 |
| ATOM | 2344 | CG2 | ILE | 159 | -3.968 | -13.361 | -16.880 | 1.00 | 0.21 |
| ATOM | 2345 | HG21 | ILE | 159 | -2.998 | -12.914 | -17.036 | 1.00 | 1.01 |
| ATOM | 2346 | HG22 | ILE | 159 | -4.556 | -13.274 | -17.781 | 1.00 | 1.01 |
| ATOM | 2347 | HG23 | ILE | 159 | -3.848 | -14.398 | -16.628 | 1.00 | 1.04 |
| ATOM | 2348 | CD1 | ILE | 159 | -5.571 | -10.356 | -15.166 | 1.00 | 0.27 |
| ATOM | 2349 | HD11 | ILE | 159 | -6.322 | -9.644 | -15.476 | 1.00 | 1.05 |

35/75

| | | | | | | | | | |
|------|------|------|-----|-----|---------|---------|---------|------|------|
| ATOM | 2350 | HD12 | ILE | 159 | -4.644 | -9.838 | -14.978 | 1.00 | 1.06 |
| ATOM | 2351 | HD13 | ILE | 159 | -5.893 | -10.848 | -14.265 | 1.00 | 1.02 |
| ATOM | 2352 | C | ILE | 159 | -6.644 | -14.162 | -16.173 | 1.00 | 0.21 |
| ATOM | 2353 | O | ILE | 159 | -7.754 | -13.700 | -16.347 | 1.00 | 0.23 |
| ATOM | 2354 | N | GLN | 160 | -6.215 | -15.168 | -16.885 | 1.00 | 0.22 |
| ATOM | 2355 | HN | GLN | 160 | -5.322 | -15.538 | -16.726 | 1.00 | 0.21 |
| ATOM | 2356 | CA | GLN | 160 | -7.097 | -15.763 | -17.930 | 1.00 | 0.27 |
| ATOM | 2357 | HA | GLN | 160 | -7.457 | -14.979 | -18.580 | 1.00 | 0.29 |
| ATOM | 2358 | CB | GLN | 160 | -6.317 | -16.786 | -18.756 | 1.00 | 0.31 |
| ATOM | 2359 | HB1 | GLN | 160 | -6.999 | -17.334 | -19.389 | 1.00 | 0.35 |
| ATOM | 2360 | HB2 | GLN | 160 | -5.809 | -17.472 | -18.093 | 1.00 | 0.30 |
| ATOM | 2361 | CG | GLN | 160 | -5.289 | -16.062 | -19.626 | 1.00 | 0.34 |
| ATOM | 2362 | HG1 | GLN | 160 | -4.606 | -15.512 | -18.997 | 1.00 | 0.92 |
| ATOM | 2363 | HG2 | GLN | 160 | -5.799 | -15.378 | -20.290 | 1.00 | 0.91 |
| ATOM | 2364 | CD | GLN | 160 | -4.508 | -17.087 | -20.451 | 1.00 | 1.11 |
| ATOM | 2365 | OE1 | GLN | 160 | -4.451 | -18.248 | -20.100 | 1.00 | 1.88 |
| ATOM | 2366 | NE2 | GLN | 160 | -3.901 | -16.704 | -21.540 | 1.00 | 1.83 |
| ATOM | 2367 | HE21 | GLN | 160 | -3.947 | -15.767 | -21.824 | 1.00 | 2.13 |
| ATOM | 2368 | HE22 | GLN | 160 | -3.398 | -17.353 | -22.075 | 1.00 | 2.46 |
| ATOM | 2369 | C | GLN | 160 | -8.290 | -16.447 | -17.261 | 1.00 | 0.28 |
| ATOM | 2370 | O | GLN | 160 | -9.386 | -16.449 | -17.779 | 1.00 | 0.31 |
| ATOM | 2371 | N | SER | 161 | -8.086 | -17.035 | -16.117 | 1.00 | 0.27 |
| ATOM | 2372 | HN | SER | 161 | -7.193 | -17.030 | -15.714 | 1.00 | 0.25 |
| ATOM | 2373 | CA | SER | 161 | -9.213 | -17.718 | -15.424 | 1.00 | 0.30 |
| ATOM | 2374 | HA | SER | 161 | -9.658 | -18.444 | -16.089 | 1.00 | 0.34 |
| ATOM | 2375 | CB | SER | 161 | -8.690 | -18.427 | -14.174 | 1.00 | 0.33 |
| ATOM | 2376 | HB1 | SER | 161 | -7.861 | -19.067 | -14.444 | 1.00 | 0.35 |
| ATOM | 2377 | HB2 | SER | 161 | -9.476 | -19.024 | -13.741 | 1.00 | 0.36 |
| ATOM | 2378 | OG | SER | 161 | -8.267 | -17.455 | -13.227 | 1.00 | 0.33 |
| ATOM | 2379 | HG | SER | 161 | -9.045 | -16.986 | -12.915 | 1.00 | 0.94 |
| ATOM | 2380 | C | SER | 161 | -10.267 | -16.684 | -15.019 | 1.00 | 0.30 |
| ATOM | 2381 | O | SER | 161 | -11.433 | -16.997 | -14.882 | 1.00 | 0.35 |
| ATOM | 2382 | N | LEU | 162 | -9.867 | -15.457 | -14.815 | 1.00 | 0.27 |
| ATOM | 2383 | HN | LEU | 162 | -8.920 | -15.225 | -14.921 | 1.00 | 0.26 |
| ATOM | 2384 | CA | LEU | 162 | -10.852 | -14.413 | -14.405 | 1.00 | 0.29 |
| ATOM | 2385 | HA | LEU | 162 | -11.637 | -14.869 | -13.821 | 1.00 | 0.33 |
| ATOM | 2386 | CB | LEU | 162 | -10.141 | -13.350 | -13.563 | 1.00 | 0.28 |
| ATOM | 2387 | HB1 | LEU | 162 | -10.802 | -12.509 | -13.411 | 1.00 | 0.29 |
| ATOM | 2388 | HB2 | LEU | 162 | -9.256 | -13.017 | -14.086 | 1.00 | 0.27 |
| ATOM | 2389 | CG | LEU | 162 | -9.736 | -13.937 | -12.206 | 1.00 | 0.30 |
| ATOM | 2390 | HG | LEU | 162 | -9.157 | -14.836 | -12.367 | 1.00 | 0.30 |
| ATOM | 2391 | CD1 | LEU | 162 | -8.883 | -12.918 | -11.450 | 1.00 | 0.33 |
| ATOM | 2392 | HD11 | LEU | 162 | -8.496 | -13.370 | -10.549 | 1.00 | 1.03 |
| ATOM | 2393 | HD12 | LEU | 162 | -9.490 | -12.063 | -11.191 | 1.00 | 1.01 |
| ATOM | 2394 | HD13 | LEU | 162 | -8.062 | -12.601 | -12.075 | 1.00 | 1.12 |
| ATOM | 2395 | CD2 | LEU | 162 | -10.980 | -14.272 | -11.374 | 1.00 | 0.33 |
| ATOM | 2396 | HD21 | LEU | 162 | -11.227 | -15.315 | -11.502 | 1.00 | 1.05 |
| ATOM | 2397 | HD22 | LEU | 162 | -11.812 | -13.664 | -11.697 | 1.00 | 1.09 |
| ATOM | 2398 | HD23 | LEU | 162 | -10.776 | -14.078 | -10.332 | 1.00 | 1.01 |
| ATOM | 2399 | C | LEU | 162 | -11.461 | -13.742 | -15.643 | 1.00 | 0.30 |
| ATOM | 2400 | O | LEU | 162 | -12.664 | -13.615 | -15.757 | 1.00 | 0.36 |
| ATOM | 2401 | N | TYR | 163 | -10.645 | -13.300 | -16.564 | 1.00 | 0.27 |
| ATOM | 2402 | HN | TYR | 163 | -9.677 | -13.404 | -16.452 | 1.00 | 0.26 |
| ATOM | 2403 | CA | TYR | 163 | -11.188 | -12.626 | -17.783 | 1.00 | 0.31 |
| ATOM | 2404 | HA | TYR | 163 | -12.144 | -12.182 | -17.549 | 1.00 | 0.33 |
| ATOM | 2405 | CB | TYR | 163 | -10.219 | -11.531 | -18.236 | 1.00 | 0.29 |
| ATOM | 2406 | HB1 | TYR | 163 | -10.562 | -11.112 | -19.170 | 1.00 | 0.32 |
| ATOM | 2407 | HB2 | TYR | 163 | -9.234 | -11.952 | -18.371 | 1.00 | 0.29 |
| ATOM | 2408 | CG | TYR | 163 | -10.162 | -10.444 | -17.190 | 1.00 | 0.25 |
| ATOM | 2409 | CD1 | TYR | 163 | -9.223 | -10.520 | -16.155 | 1.00 | 0.23 |
| ATOM | 2410 | HD1 | TYR | 163 | -8.545 | -11.359 | -16.103 | 1.00 | 0.23 |
| ATOM | 2411 | CD2 | TYR | 163 | -11.042 | -9.357 | -17.258 | 1.00 | 0.27 |
| ATOM | 2412 | HD2 | TYR | 163 | -11.767 | -9.298 | -18.056 | 1.00 | 0.30 |
| ATOM | 2413 | CE1 | TYR | 163 | -9.164 | -9.511 | -15.187 | 1.00 | 0.24 |
| ATOM | 2414 | HE1 | TYR | 163 | -8.439 | -9.571 | -14.388 | 1.00 | 0.25 |
| ATOM | 2415 | CE2 | TYR | 163 | -10.984 | -8.348 | -16.289 | 1.00 | 0.27 |
| ATOM | 2416 | HE2 | TYR | 163 | -11.663 | -7.510 | -16.340 | 1.00 | 0.30 |
| ATOM | 2417 | CZ | TYR | 163 | -10.044 | -8.425 | -15.253 | 1.00 | 0.27 |
| ATOM | 2418 | OH | TYR | 163 | -9.985 | -7.430 | -14.299 | 1.00 | 0.31 |
| ATOM | 2419 | HH | TYR | 163 | -10.344 | -7.782 | -13.481 | 1.00 | 0.99 |
| ATOM | 2420 | C | TYR | 163 | -11.367 | -13.647 | -18.909 | 1.00 | 0.37 |
| ATOM | 2421 | O | TYR | 163 | -11.953 | -13.357 | -19.933 | 1.00 | 0.43 |
| ATOM | 2422 | N | GLY | 164 | -10.865 | -14.836 | -18.729 | 1.00 | 0.38 |
| ATOM | 2423 | HN | GLY | 164 | -10.394 | -15.046 | -17.896 | 1.00 | 0.35 |
| ATOM | 2424 | CA | GLY | 164 | -11.001 | -15.877 | -19.789 | 1.00 | 0.47 |
| ATOM | 2425 | HA1 | GLY | 164 | -11.851 | -15.651 | -20.413 | 1.00 | 0.53 |
| ATOM | 2426 | HA2 | GLY | 164 | -11.851 | -15.651 | -20.413 | 1.00 | 0.53 |

36/75

| | | | | | | | | | |
|--------|------|------|-----|-----|--------|---------|---------|------|------|
| ATOM | 2427 | C | GLY | 164 | -9.735 | -15.902 | -20.648 | 1.00 | 0.55 |
| ATOM | 2428 | O | GLY | 164 | -9.761 | -15.580 | -21.819 | 1.00 | 1.01 |
| TER | 2429 | | GLY | 164 | | | | | |
| HETATM | 2430 | ZN | ZN | 166 | -0.218 | -6.515 | -2.613 | 1.00 | 0.24 |
| HETATM | 2431 | ZN | ZN | 167 | -3.506 | 6.833 | -0.714 | 1.00 | 0.97 |
| HETATM | 2432 | CA | CA | 168 | 6.060 | 3.350 | 3.030 | 1.00 | 0.23 |
| HETATM | 2433 | C1 | WAY | 169 | 2.180 | -4.315 | 1.627 | 0.00 | 0.30 |
| HETATM | 2434 | C2 | WAY | 169 | 0.865 | -4.629 | 1.215 | 0.00 | 0.33 |
| HETATM | 2435 | 1CE1 | WAY | 169 | -0.170 | -4.517 | 2.143 | 0.00 | 0.38 |
| HETATM | 2436 | 1CZ | WAY | 169 | 0.074 | -4.157 | 3.457 | 0.00 | 0.40 |
| HETATM | 2437 | 1CE2 | WAY | 169 | 1.355 | -3.807 | 3.841 | 0.00 | 0.38 |
| HETATM | 2438 | C6 | WAY | 169 | 2.395 | -3.805 | 2.922 | 0.00 | 0.33 |
| HETATM | 2439 | 1HE1 | WAY | 169 | -1.190 | -4.713 | 1.839 | 0.00 | 0.42 |
| HETATM | 2440 | 1HZ | WAY | 169 | -0.734 | -4.151 | 4.173 | 0.00 | 0.45 |
| HETATM | 2441 | 1HE2 | WAY | 169 | 1.535 | -3.534 | 4.872 | 0.00 | 0.42 |
| HETATM | 2442 | C10 | WAY | 169 | 0.444 | -5.080 | -0.136 | 0.00 | 0.36 |
| HETATM | 2443 | O11 | WAY | 169 | 0.467 | -6.264 | -0.463 | 0.00 | 0.58 |
| HETATM | 2444 | N12 | WAY | 169 | -0.019 | -4.195 | -1.032 | 0.00 | 0.61 |
| HETATM | 2445 | O13 | WAY | 169 | -0.045 | -4.608 | -2.371 | 0.00 | 0.68 |
| HETATM | 2446 | H14 | WAY | 169 | -0.357 | -3.297 | -0.743 | 0.00 | 0.88 |
| HETATM | 2447 | H15 | WAY | 169 | -0.953 | -4.727 | -2.645 | 0.00 | 1.13 |
| HETATM | 2448 | 1CH1 | WAY | 169 | 3.728 | -3.247 | 3.360 | 0.00 | 0.37 |
| HETATM | 2449 | 1HH1 | WAY | 169 | 3.702 | -2.162 | 3.422 | 0.00 | 1.07 |
| HETATM | 2450 | 1HH2 | WAY | 169 | 4.519 | -3.516 | 2.664 | 0.00 | 1.06 |
| HETATM | 2451 | 1HH3 | WAY | 169 | 4.013 | -3.623 | 4.339 | 0.00 | 1.11 |
| HETATM | 2452 | N20 | WAY | 169 | 3.274 | -4.485 | 0.819 | 0.00 | 0.29 |
| HETATM | 2453 | S21 | WAY | 169 | 3.865 | -3.175 | 0.021 | 0.00 | 0.25 |
| HETATM | 2454 | 2CB | WAY | 169 | 3.882 | -5.812 | 0.684 | 0.00 | 0.32 |
| HETATM | 2455 | 2CE1 | WAY | 169 | 7.334 | -6.241 | 2.178 | 0.00 | 1.09 |
| HETATM | 2456 | 2CZ | WAY | 169 | 6.971 | -6.520 | 3.488 | 0.00 | 0.53 |
| HETATM | 2457 | N25 | WAY | 169 | 5.697 | -6.659 | 3.876 | 0.00 | 1.47 |
| HETATM | 2458 | 2CD2 | WAY | 169 | 4.747 | -6.451 | 2.954 | 0.00 | 1.37 |
| HETATM | 2459 | C27 | WAY | 169 | 5.010 | -6.084 | 1.640 | 0.00 | 0.36 |
| HETATM | 2460 | 2CD1 | WAY | 169 | 6.338 | -5.982 | 1.250 | 0.00 | 1.14 |
| HETATM | 2461 | 2HE1 | WAY | 169 | 8.374 | -6.224 | 1.881 | 0.00 | 1.94 |
| HETATM | 2462 | 2HZ | WAY | 169 | 7.752 | -6.630 | 4.227 | 0.00 | 0.61 |
| HETATM | 2463 | 2HD2 | WAY | 169 | 3.708 | -6.570 | 3.227 | 0.00 | 2.23 |
| HETATM | 2464 | 2HD1 | WAY | 169 | 6.599 | -5.706 | 0.239 | 0.00 | 2.05 |
| HETATM | 2465 | 2HB1 | WAY | 169 | 4.245 | -5.905 | -0.339 | 0.00 | 0.31 |
| HETATM | 2466 | 2HB2 | WAY | 169 | 3.095 | -6.552 | 0.832 | 0.00 | 0.34 |
| HETATM | 2467 | C35 | WAY | 169 | 4.187 | -3.617 | -1.665 | 0.00 | 0.23 |
| HETATM | 2468 | 3CD1 | WAY | 169 | 3.310 | -3.216 | -2.661 | 0.00 | 0.25 |
| HETATM | 2469 | 3CE1 | WAY | 169 | 3.622 | -3.465 | -3.992 | 0.00 | 0.27 |
| HETATM | 2470 | C38 | WAY | 169 | 4.769 | -4.183 | -4.326 | 0.00 | 0.24 |
| HETATM | 2471 | 3CE2 | WAY | 169 | 5.602 | -4.644 | -3.308 | 0.00 | 0.23 |
| HETATM | 2472 | 3CD2 | WAY | 169 | 5.315 | -4.359 | -1.979 | 0.00 | 0.23 |
| HETATM | 2473 | 3HD1 | WAY | 169 | 2.392 | -2.714 | -2.389 | 0.00 | 0.29 |
| HETATM | 2474 | 3HE1 | WAY | 169 | 2.961 | -3.091 | -4.758 | 0.00 | 0.31 |
| HETATM | 2475 | 3HE2 | WAY | 169 | 6.481 | -5.228 | -3.535 | 0.00 | 0.26 |
| HETATM | 2476 | 3HD2 | WAY | 169 | 5.959 | -4.707 | -1.184 | 0.00 | 0.27 |
| HETATM | 2477 | O45 | WAY | 169 | 5.078 | -4.439 | -5.664 | 0.00 | 0.27 |
| HETATM | 2478 | 3CH | WAY | 169 | 6.245 | -5.202 | -5.904 | 0.00 | 0.28 |
| HETATM | 2479 | 3HH1 | WAY | 169 | 6.379 | -5.372 | -6.973 | 0.00 | 0.31 |
| HETATM | 2480 | 3HH2 | WAY | 169 | 6.178 | -6.172 | -5.407 | 0.00 | 0.28 |
| HETATM | 2481 | 3HH3 | WAY | 169 | 7.127 | -4.683 | -5.526 | 0.00 | 0.29 |
| HETATM | 2482 | O50 | WAY | 169 | 5.123 | -2.847 | 0.614 | 0.00 | 0.27 |
| HETATM | 2483 | O51 | WAY | 169 | 2.834 | -2.186 | 0.004 | 0.00 | 0.25 |
| END | | | | | | | | | |

37/75

| | Atom Type | Res. | | X | Y | Z | Occ. | B | MOL. |
|------|--------------|---------|----|--------|--------|--------|------|-------|------|
| ATOM | 1 | CB THR | 7 | 73.468 | 27.410 | 6.079 | 1.00 | 42.70 | A_13 |
| ATOM | 2 | OG1 THR | 7 | 72.149 | 27.911 | 6.358 | 1.00 | 37.82 | A_13 |
| ATOM | 4 | CG2 THR | 7 | 73.843 | 26.297 | 7.068 | 1.00 | 25.79 | A_13 |
| ATOM | 5 | C THR | 7 | 75.936 | 28.076 | 6.227 | 1.00 | 28.29 | A_13 |
| ATOM | 6 | O THR | 7 | 76.497 | 28.090 | 7.332 | 1.00 | 22.94 | A_13 |
| ATOM | 9 | N THR | 7 | 74.360 | 29.396 | 4.862 | 1.00 | 20.25 | A_13 |
| ATOM | 11 | CA THR | 7 | 74.501 | 28.593 | 6.099 | 1.00 | 21.49 | A_13 |
| ATOM | 12 | N LEU | 8 | 76.547 | 27.691 | 5.099 | 1.00 | 32.90 | A_13 |
| ATOM | 14 | CA LEU | 8 | 77.915 | 27.150 | 5.105 | 1.00 | 31.85 | A_13 |
| ATOM | 15 | CB LEU | 8 | 77.952 | 25.759 | 4.438 | 1.00 | 21.38 | A_13 |
| ATOM | 16 | CG LEU | 8 | 78.016 | 25.576 | 2.910 | 1.00 | 29.31 | A_13 |
| ATOM | 17 | CD1 LEU | 8 | 79.463 | 25.509 | 2.425 | 1.00 | 16.78 | A_13 |
| ATOM | 18 | CD2 LEU | 8 | 77.334 | 24.292 | 2.527 | 1.00 | 23.37 | A_13 |
| ATOM | 19 | C LEU | 8 | 78.956 | 28.070 | 4.465 | 1.00 | 24.01 | A_13 |
| ATOM | 20 | O LEU | 8 | 78.835 | 28.415 | 3.293 | 1.00 | 26.18 | A_13 |
| ATOM | 21 | N LYS | 9 | 79.980 | 28.424 | 5.251 | 1.00 | 36.26 | A_13 |
| ATOM | 23 | CA LYS | 9 | 81.106 | 29.298 | 4.867 | 1.00 | 23.24 | A_13 |
| ATOM | 24 | CB LYS | 9 | 82.438 | 28.521 | 4.977 | 1.00 | 25.52 | A_13 |
| ATOM | 25 | CG LYS | 9 | 82.767 | 27.570 | 3.815 | 1.00 | 19.05 | A_13 |
| ATOM | 26 | CD LYS | 9 | 83.661 | 28.243 | 2.753 | 1.00 | 31.69 | A_13 |
| ATOM | 27 | CE LYS | 9 | 83.451 | 27.688 | 1.323 | 1.00 | 25.30 | A_13 |
| ATOM | 28 | NZ LYS | 9 | 82.056 | 27.938 | 0.797 | 1.00 | 20.65 | A_13 |
| ATOM | 32 | C LYS | 9 | 81.042 | 30.073 | 3.526 | 1.00 | 31.41 | A_13 |
| ATOM | 33 | O LYS | 9 | 80.764 | 29.505 | 2.466 | 1.00 | 22.31 | A_13 |
| ATOM | 34 | N TRP | 10 | 81.327 | 31.372 | 3.573 | 1.00 | 15.84 | A_13 |
| ATOM | 36 | CA TRP | 10 | 81.312 | 32.172 | 2.361 | 1.00 | 10.58 | A_13 |
| ATOM | 37 | CB TRP | 10 | 81.636 | 33.620 | 2.680 | 1.00 | 21.39 | A_13 |
| ATOM | 38 | CG TRP | 10 | 80.529 | 34.337 | 3.343 | 1.00 | 22.84 | A_13 |
| ATOM | 39 | CD2 TRP | 10 | 79.479 | 35.074 | 2.697 | 1.00 | 20.41 | A_13 |
| ATOM | 40 | CE2 TRP | 10 | 78.676 | 35.631 | 3.718 | 1.00 | 24.50 | A_13 |
| ATOM | 41 | CE3 TRP | 10 | 79.142 | 35.320 | 1.357 | 1.00 | 13.29 | A_13 |
| ATOM | 42 | CD1 TRP | 10 | 80.327 | 34.469 | 4.682 | 1.00 | 13.40 | A_13 |
| ATOM | 43 | NE1 TRP | 10 | 79.220 | 35.253 | 4.919 | 1.00 | 18.40 | A_13 |
| ATOM | 45 | CZ2 TRP | 10 | 77.550 | 36.418 | 3.442 | 1.00 | 12.63 | A_13 |
| ATOM | 46 | CZ3 TRP | 10 | 78.021 | 36.105 | 1.083 | 1.00 | 19.89 | A_13 |
| ATOM | 47 | CH2 TRP | 10 | 77.242 | 36.641 | 2.120 | 1.00 | 13.62 | A_13 |
| ATOM | 48 | C TRP | 10 | 82.377 | 31.594 | 1.455 | 1.00 | 22.95 | A_13 |
| ATOM | 49 | O TRP | 10 | 83.450 | 31.221 | 1.920 | 1.00 | 16.28 | A_13 |
| ATOM | 50 | N SER | 11 | 82.087 | 31.533 | 0.167 | 1.00 | 14.81 | A_13 |
| ATOM | 52 | CA SER | 11 | 83.017 | 30.975 | -0.801 | 1.00 | 19.50 | A_13 |
| ATOM | 53 | CB SER | 11 | 82.282 | 30.596 | -2.086 | 1.00 | 24.36 | A_13 |
| ATOM | 54 | OG SER | 11 | 81.605 | 29.353 | -1.958 | 1.00 | 40.49 | A_13 |
| ATOM | 56 | C SER | 11 | 84.190 | 31.867 | -1.134 | 1.00 | 16.53 | A_13 |
| ATOM | 57 | O SER | 11 | 85.132 | 31.423 | -1.779 | 1.00 | 23.48 | A_13 |
| ATOM | 58 | N LYS | 12 | 84.153 | 33.113 | -0.686 | 1.00 | 12.50 | A_13 |
| ATOM | 60 | CA LYS | 12 | 85.232 | 34.057 | -0.961 | 1.00 | 17.05 | A_13 |
| ATOM | 61 | CB LYS | 12 | 84.741 | 35.168 | -1.891 | 1.00 | 17.32 | A_13 |
| ATOM | 62 | CG LYS | 12 | 83.526 | 35.898 | -1.350 | 1.00 | 18.49 | A_13 |
| ATOM | 63 | CD LYS | 12 | 82.788 | 36.644 | -2.446 | 1.00 | 18.29 | A_13 |
| ATOM | 64 | CE LYS | 12 | 81.534 | 37.282 | -1.888 | 1.00 | 18.44 | A_13 |
| ATOM | 65 | NZ LYS | 12 | 80.805 | 38.094 | -2.895 | 1.00 | 16.65 | A_13 |
| ATOM | 69 | C LYS | 12 | 85.687 | 34.662 | 0.344 | 1.00 | 11.16 | A_13 |
| ATOM | 70 | O LYS | 12 | 84.946 | 34.637 | 1.319 | 1.00 | 12.63 | A_13 |
| ATOM | 71 | N MET | 13 | 85.915 | 35.185 | 0.355 | 1.00 | 15.52 | A_13 |
| ATOM | 73 | CA MET | 13 | 87.516 | 35.801 | 1.537 | 1.00 | 11.04 | A_13 |
| ATOM | 74 | CB MET | 13 | 89.028 | 35.547 | 1.565 | 1.00 | 16.57 | A_13 |
| ATOM | 75 | CG MET | 13 | 89.431 | 34.082 | 1.707 | 1.00 | 20.92 | A_13 |
| ATOM | 76 | SD MET | 13 | 88.905 | 33.235 | 3.227 | 1.00 | 20.10 | A_13 |
| ATOM | 77 | CE MET | 13 | 87.486 | 32.313 | 2.604 | 1.00 | 16.29 | A_13 |
| ATOM | 78 | C MET | 13 | 87.258 | 37.296 | 1.572 | 1.00 | 13.23 | A_13 |
| ATOM | 79 | O MET | 13 | 87.247 | 37.916 | 2.634 | 1.00 | 22.80 | A_13 |
| ATOM | 80 | N ASN | 14 | 87.111 | 37.875 | 0.389 | 1.00 | 15.02 | A_13 |
| ATOM | 82 | CA ASN | 14 | 86.853 | 39.294 | 0.241 | 1.00 | 33.02 | A_13 |
| ATOM | 83 | CB ASN | 14 | 87.445 | 39.801 | -1.082 | 1.00 | 19.42 | A_13 |
| ATOM | 84 | CG ASN | 14 | 88.925 | 39.482 | -1.217 | 1.00 | 30.32 | A_13 |
| ATOM | 85 | OD1 ASN | 14 | 89.343 | 38.341 | -1.031 | 1.00 | 30.12 | A_13 |
| ATOM | 86 | ND2 ASN | 14 | 89.723 | 40.489 | -1.549 | 1.00 | 28.22 | A_13 |
| ATOM | 89 | C ASN | 14 | 85.337 | 39.482 | 0.277 | 1.00 | 27.58 | A_13 |
| ATOM | 90 | O ASN | 14 | 84.606 | 38.935 | -0.568 | 1.00 | 28.01 | A_13 |
| ATOM | 91 | N LEU | 15 | 84.868 | 40.212 | 1.287 | 1.00 | 19.06 | A_13 |
| ATOM | 93 | CA LEU | 15 | 83.444 | 40.450 | 1.459 | 1.00 | 20.03 | A_13 |
| ATOM | 94 | CB LEU | 15 | 82.930 | 39.690 | 2.691 | 1.00 | 19.55 | A_13 |
| ATOM | 95 | CG LEU | 15 | 83.027 | 38.166 | 2.593 | 1.00 | 19.02 | A_13 |
| ATOM | 96 | CD1 LEU | 15 | 83.216 | 37.555 | 3.962 | 1.00 | 17.48 | A_13 |
| ATOM | 97 | CD2 LEU | 15 | 81.799 | 37.604 | 1.903 | 1.00 | 23.43 | A_13 |
| ATOM | 98 | C LEU | 15 | 83.161 | 41.928 | 1.609 | 1.00 | 19.52 | A_13 |
| ATOM | 99 | O LEU | 15 | 83.980 | 42.676 | 2.130 | 1.00 | 15.98 | A_13 |

FIG. 5

38 / 75

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 100 | N | THR | 16 | 81.983 | 42.343 | 1.162 | 1.00 | 21.22 | A_13 |
| ATOM | 102 | CA | THR | 16 | 81.578 | 43.736 | 1.252 | 1.00 | 10.00 | A_13 |
| ATOM | 103 | CB | THR | 16 | 81.194 | 44.257 | -0.109 | 1.00 | 10.00 | A_13 |
| ATOM | 104 | OG1 | THR | 16 | 80.225 | 43.370 | -0.681 | 1.00 | 22.43 | A_13 |
| ATOM | 106 | CG2 | THR | 16 | 82.427 | 44.383 | -1.009 | 1.00 | 15.42 | A_13 |
| ATOM | 107 | C | THR | 16 | 80.368 | 43.869 | 2.184 | 1.00 | 14.48 | A_13 |
| ATOM | 108 | O | THR | 16 | 79.647 | 42.897 | 2.445 | 1.00 | 15.74 | A_13 |
| ATOM | 109 | N | TYR | 17 | 80.176 | 45.065 | 2.716 | 1.00 | 15.89 | A_13 |
| ATOM | 111 | CA | TYR | 17 | 79.064 | 45.340 | 3.604 | 1.00 | 13.19 | A_13 |
| ATOM | 112 | CB | TYR | 17 | 79.480 | 45.195 | 5.067 | 1.00 | 21.42 | A_13 |
| ATOM | 113 | CG | TYR | 17 | 80.448 | 46.236 | 5.580 | 1.00 | 26.23 | A_13 |
| ATOM | 114 | CD1 | TYR | 17 | 81.824 | 46.081 | 5.412 | 1.00 | 16.37 | A_13 |
| ATOM | 115 | CE1 | TYR | 17 | 82.724 | 46.981 | 5.988 | 1.00 | 12.90 | A_13 |
| ATOM | 116 | CD2 | TYR | 17 | 79.990 | 47.329 | 6.331 | 1.00 | 17.15 | A_13 |
| ATOM | 117 | CE2 | TYR | 17 | 80.880 | 48.235 | 6.912 | 1.00 | 24.15 | A_13 |
| ATOM | 118 | CZ | TYR | 17 | 82.244 | 48.057 | 6.743 | 1.00 | 23.38 | A_13 |
| ATOM | 119 | OH | TYR | 17 | 83.121 | 48.942 | 7.343 | 1.00 | 19.47 | A_13 |
| ATOM | 121 | C | TYR | 17 | 78.573 | 46.740 | 3.343 | 1.00 | 10.00 | A_13 |
| ATOM | 122 | O | TYR | 17 | 79.298 | 47.559 | 2.782 | 1.00 | 19.27 | A_13 |
| ATOM | 123 | N | ARG | 18 | 77.349 | 47.019 | 3.762 | 1.00 | 18.52 | A_13 |
| ATOM | 125 | CA | ARG | 18 | 76.762 | 48.332 | 3.577 | 1.00 | 10.00 | A_13 |
| ATOM | 126 | CB | ARG | 18 | 75.970 | 48.363 | 2.274 | 1.00 | 10.00 | A_13 |
| ATOM | 127 | CG | ARG | 18 | 75.134 | 49.619 | 2.094 | 1.00 | 14.01 | A_13 |
| ATOM | 128 | CD | ARG | 18 | 74.266 | 49.524 | 0.846 | 1.00 | 13.91 | A_13 |
| ATOM | 129 | NE | ARG | 18 | 73.298 | 50.615 | 0.782 | 1.00 | 13.55 | A_13 |
| ATOM | 131 | CZ | ARG | 18 | 72.165 | 50.571 | 0.092 | 1.00 | 10.00 | A_13 |
| ATOM | 132 | NH1 | ARG | 18 | 71.855 | 49.488 | -0.602 | 1.00 | 14.30 | A_13 |
| ATOM | 135 | NH2 | ARG | 18 | 71.331 | 51.604 | 0.125 | 1.00 | 28.79 | A_13 |
| ATOM | 138 | C | ARG | 18 | 75.842 | 48.640 | 4.741 | 1.00 | 10.65 | A_13 |
| ATOM | 139 | O | ARG | 18 | 75.037 | 47.796 | 5.141 | 1.00 | 12.86 | A_13 |
| ATOM | 140 | N | ILE | 19 | 76.014 | 49.814 | 5.332 | 1.00 | 25.54 | A_13 |
| ATOM | 142 | CA | ILE | 19 | 75.169 | 50.265 | 6.436 | 1.00 | 24.52 | A_13 |
| ATOM | 143 | CB | ILE | 19 | 75.944 | 51.236 | 7.350 | 1.00 | 18.37 | A_13 |
| ATOM | 144 | CG2 | ILE | 19 | 75.034 | 51.765 | 8.485 | 1.00 | 13.87 | A_13 |
| ATOM | 145 | CG1 | ILE | 19 | 77.204 | 50.545 | 7.888 | 1.00 | 27.67 | A_13 |
| ATOM | 146 | CD1 | ILE | 19 | 78.203 | 51.501 | 8.557 | 1.00 | 22.81 | A_13 |
| ATOM | 147 | C | ILE | 19 | 74.062 | 51.027 | 5.698 | 1.00 | 21.11 | A_13 |
| ATOM | 148 | O | ILE | 19 | 74.261 | 52.179 | 5.300 | 1.00 | 10.00 | A_13 |
| ATOM | 149 | N | VAL | 20 | 72.916 | 50.378 | 5.487 | 1.00 | 19.76 | A_13 |
| ATOM | 151 | CA | VAL | 20 | 71.829 | 51.014 | 4.735 | 1.00 | 18.20 | A_13 |
| ATOM | 152 | CB | VAL | 20 | 70.774 | 49.983 | 4.193 | 1.00 | 15.42 | A_13 |
| ATOM | 153 | CG1 | VAL | 20 | 71.384 | 48.570 | 4.088 | 1.00 | 10.00 | A_13 |
| ATOM | 154 | CG2 | VAL | 20 | 69.496 | 50.030 | 4.992 | 1.00 | 18.62 | A_13 |
| ATOM | 155 | C | VAL | 20 | 71.175 | 52.206 | 5.443 | 1.00 | 11.67 | A_13 |
| ATOM | 156 | O | VAL | 20 | 70.652 | 53.110 | 4.798 | 1.00 | 18.36 | A_13 |
| ATOM | 157 | N | ASN | 21 | 71.153 | 52.187 | 6.773 | 1.00 | 10.94 | A_13 |
| ATOM | 159 | CA | ASN | 21 | 70.609 | 53.316 | 7.544 | 1.00 | 11.99 | A_13 |
| ATOM | 160 | CB | ASN | 21 | 69.078 | 53.307 | 7.675 | 1.00 | 10.00 | A_13 |
| ATOM | 161 | CG | ASN | 21 | 68.533 | 51.978 | 8.107 | 1.00 | 14.93 | A_13 |
| ATOM | 162 | OD1 | ASN | 21 | 67.627 | 51.449 | 7.486 | 1.00 | 21.54 | A_13 |
| ATOM | 163 | ND2 | ASN | 21 | 69.105 | 51.408 | 9.148 | 1.00 | 10.00 | A_13 |
| ATOM | 166 | C | ASN | 21 | 71.291 | 53.382 | 8.897 | 1.00 | 18.90 | A_13 |
| ATOM | 167 | O | ASN | 21 | 72.006 | 52.447 | 9.283 | 1.00 | 12.49 | A_13 |
| ATOM | 168 | N | TYR | 22 | 71.053 | 54.471 | 9.618 | 1.00 | 17.47 | A_13 |
| ATOM | 170 | CA | TYR | 22 | 71.681 | 54.708 | 10.910 | 1.00 | 24.85 | A_13 |
| ATOM | 171 | CB | TYR | 22 | 72.556 | 55.954 | 10.818 | 1.00 | 13.52 | A_13 |
| ATOM | 172 | CG | TYR | 22 | 73.791 | 55.748 | 9.991 | 1.00 | 10.00 | A_13 |
| ATOM | 173 | CD1 | TYR | 22 | 75.033 | 55.600 | 10.598 | 1.00 | 14.05 | A_13 |
| ATOM | 174 | CE1 | TYR | 22 | 76.180 | 55.370 | 9.841 | 1.00 | 13.69 | A_13 |
| ATOM | 175 | CD2 | TYR | 22 | 73.717 | 55.663 | 8.608 | 1.00 | 10.00 | A_13 |
| ATOM | 176 | CE2 | TYR | 22 | 74.848 | 55.432 | 7.847 | 1.00 | 17.10 | A_13 |
| ATOM | 177 | CZ | TYR | 22 | 76.077 | 55.288 | 8.476 | 1.00 | 14.43 | A_13 |
| ATOM | 178 | OH | TYR | 22 | 77.204 | 55.072 | 7.737 | 1.00 | 10.00 | A_13 |
| ATOM | 180 | C | TYR | 22 | 70.726 | 54.862 | 12.076 | 1.00 | 25.95 | A_13 |
| ATOM | 181 | O | TYR | 22 | 69.593 | 55.311 | 11.916 | 1.00 | 10.00 | A_13 |
| ATOM | 182 | N | THR | 23 | 71.187 | 54.483 | 13.259 | 1.00 | 20.30 | A_13 |
| ATOM | 184 | CA | THR | 23 | 70.367 | 54.606 | 14.450 | 1.00 | 29.11 | A_13 |
| ATOM | 185 | CB | THR | 23 | 70.821 | 53.635 | 15.584 | 1.00 | 10.90 | A_13 |
| ATOM | 186 | OG1 | THR | 23 | 70.136 | 53.968 | 16.792 | 1.00 | 10.00 | A_13 |
| ATOM | 188 | CG2 | THR | 23 | 72.328 | 53.752 | 15.852 | 1.00 | 16.51 | A_13 |
| ATOM | 189 | C | THR | 23 | 70.459 | 56.038 | 14.959 | 1.00 | 18.14 | A_13 |
| ATOM | 190 | O | THR | 23 | 71.360 | 56.785 | 14.575 | 1.00 | 10.00 | A_13 |
| ATOM | 191 | N | PRO | 24 | 69.433 | 56.487 | 15.691 | 1.00 | 12.76 | A_13 |
| ATOM | 192 | CD | PRO | 24 | 68.061 | 55.950 | 15.716 | 1.00 | 15.26 | A_13 |
| ATOM | 193 | CA | PRO | 24 | 69.453 | 57.844 | 16.232 | 1.00 | 22.70 | A_13 |
| ATOM | 194 | CB | PRO | 24 | 67.985 | 58.086 | 16.585 | 1.00 | 28.52 | A_13 |
| ATOM | 195 | CG | PRO | 24 | 67.448 | 56.706 | 16.841 | 1.00 | 15.78 | A_13 |

39/75

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 196 | C | PRO | 24 | 70.346 | 57.945 | 17.475 | 1.00 | 24.52 | A_13 |
| ATOM | 197 | O | PRO | 24 | 70.790 | 59.040 | 17.831 | 1.00 | 10.00 | A_13 |
| ATOM | 198 | N | ASP | 25 | 70.614 | 56.797 | 18.105 | 1.00 | 11.82 | A_13 |
| ATOM | 200 | CA | ASP | 25 | 71.416 | 56.721 | 19.336 | 1.00 | 12.31 | A_13 |
| ATOM | 201 | CB | ASP | 25 | 71.339 | 55.317 | 19.917 | 1.00 | 25.26 | A_13 |
| ATOM | 202 | CG | ASP | 25 | 69.927 | 54.782 | 19.977 | 1.00 | 10.00 | A_13 |
| ATOM | 203 | OD1 | ASP | 25 | 69.783 | 53.567 | 20.159 | 1.00 | 20.90 | A_13 |
| ATOM | 204 | OD2 | ASP | 25 | 68.960 | 55.558 | 19.841 | 1.00 | 18.45 | A_13 |
| ATOM | 205 | C | ASP | 25 | 72.891 | 57.113 | 19.286 | 1.00 | 14.34 | A_13 |
| ATOM | 206 | O | ASP | 25 | 73.449 | 57.511 | 20.301 | 1.00 | 11.77 | A_13 |
| ATOM | 207 | N | MET | 26 | 73.546 | 56.873 | 18.157 | 1.00 | 20.78 | A_13 |
| ATOM | 209 | CA | MET | 26 | 74.960 | 57.208 | 18.010 | 1.00 | 20.03 | A_13 |
| ATOM | 210 | CB | MET | 26 | 75.791 | 55.928 | 17.916 | 1.00 | 13.86 | A_13 |
| ATOM | 211 | CG | MET | 26 | 75.966 | 55.181 | 19.231 | 1.00 | 19.00 | A_13 |
| ATOM | 212 | SD | MET | 26 | 76.043 | 53.404 | 18.941 | 1.00 | 14.67 | A_13 |
| ATOM | 213 | CE | MET | 26 | 77.737 | 53.223 | 18.385 | 1.00 | 19.74 | A_13 |
| ATOM | 214 | C | MET | 26 | 75.157 | 58.047 | 16.754 | 1.00 | 13.32 | A_13 |
| ATOM | 215 | O | MET | 26 | 74.274 | 58.086 | 15.900 | 1.00 | 16.81 | A_13 |
| ATOM | 216 | N | THR | 27 | 76.285 | 58.749 | 16.656 | 1.00 | 10.29 | A_13 |
| ATOM | 218 | CA | THR | 27 | 76.568 | 59.564 | 15.470 | 1.00 | 17.00 | A_13 |
| ATOM | 219 | CB | THR | 27 | 77.710 | 60.596 | 15.700 | 1.00 | 11.79 | A_13 |
| ATOM | 220 | OG1 | THR | 27 | 78.969 | 59.921 | 15.729 | 1.00 | 23.77 | A_13 |
| ATOM | 222 | CG2 | THR | 27 | 77.519 | 61.342 | 17.020 | 1.00 | 21.98 | A_13 |
| ATOM | 223 | C | THR | 27 | 76.996 | 58.634 | 14.347 | 1.00 | 13.37 | A_13 |
| ATOM | 224 | O | THR | 27 | 77.411 | 57.500 | 14.608 | 1.00 | 11.05 | A_13 |
| ATOM | 225 | N | HIS | 28 | 76.972 | 59.124 | 13.113 | 1.00 | 10.00 | A_13 |
| ATOM | 227 | CA | HIS | 28 | 77.362 | 58.300 | 11.980 | 1.00 | 10.96 | A_13 |
| ATOM | 228 | CB | HIS | 28 | 77.240 | 59.071 | 10.657 | 1.00 | 16.07 | A_13 |
| ATOM | 229 | CG | HIS | 28 | 75.829 | 59.382 | 10.264 | 1.00 | 15.53 | A_13 |
| ATOM | 230 | CD2 | HIS | 28 | 74.707 | 59.531 | 11.016 | 1.00 | 21.47 | A_13 |
| ATOM | 231 | ND1 | HIS | 28 | 75.440 | 59.597 | 8.959 | 1.00 | 30.32 | A_13 |
| ATOM | 233 | CE1 | HIS | 28 | 74.149 | 59.868 | 8.920 | 1.00 | 19.38 | A_13 |
| ATOM | 234 | NE2 | HIS | 28 | 73.680 | 59.833 | 10.160 | 1.00 | 29.43 | A_13 |
| ATOM | 236 | C | HIS | 28 | 78.769 | 57.735 | 12.151 | 1.00 | 14.80 | A_13 |
| ATOM | 237 | O | HIS | 28 | 79.005 | 56.568 | 11.851 | 1.00 | 28.24 | A_13 |
| ATOM | 238 | N | SER | 29 | 79.703 | 58.548 | 12.634 | 1.00 | 14.00 | A_13 |
| ATOM | 240 | CA | SER | 29 | 81.068 | 58.070 | 12.854 | 1.00 | 19.57 | A_13 |
| ATOM | 241 | CB | SER | 29 | 82.001 | 59.219 | 13.242 | 1.00 | 17.84 | A_13 |
| ATOM | 242 | OG | SER | 29 | 82.383 | 59.936 | 12.084 | 1.00 | 28.25 | A_13 |
| ATOM | 244 | C | SER | 29 | 81.134 | 56.983 | 13.917 | 1.00 | 15.23 | A_13 |
| ATOM | 245 | O | SER | 29 | 81.818 | 55.973 | 13.733 | 1.00 | 13.73 | A_13 |
| ATOM | 246 | N | GLU | 30 | 80.428 | 57.182 | 15.027 | 1.00 | 27.71 | A_13 |
| ATOM | 248 | CA | GLU | 30 | 80.430 | 56.186 | 16.100 | 1.00 | 23.60 | A_13 |
| ATOM | 249 | CB | GLU | 30 | 79.571 | 56.635 | 17.289 | 1.00 | 21.72 | A_13 |
| ATOM | 250 | CG | GLU | 30 | 80.048 | 57.913 | 17.973 | 1.00 | 24.07 | A_13 |
| ATOM | 251 | CD | GLU | 30 | 79.205 | 58.279 | 19.185 | 1.00 | 21.06 | A_13 |
| ATOM | 252 | OE1 | GLU | 30 | 79.784 | 58.660 | 20.218 | 1.00 | 46.95 | A_13 |
| ATOM | 253 | OE2 | GLU | 30 | 77.963 | 58.185 | 19.119 | 1.00 | 18.27 | A_13 |
| ATOM | 254 | C | GLU | 30 | 79.895 | 54.877 | 15.553 | 1.00 | 18.75 | A_13 |
| ATOM | 255 | O | GLU | 30 | 80.456 | 53.809 | 15.815 | 1.00 | 13.06 | A_13 |
| ATOM | 256 | N | VAL | 31 | 78.839 | 54.970 | 14.746 | 1.00 | 16.23 | A_13 |
| ATOM | 258 | CA | VAL | 31 | 78.225 | 53.781 | 14.146 | 1.00 | 22.33 | A_13 |
| ATOM | 259 | CB | VAL | 31 | 76.899 | 54.135 | 13.390 | 1.00 | 23.53 | A_13 |
| ATOM | 260 | CG1 | VAL | 31 | 76.384 | 52.920 | 12.628 | 1.00 | 14.39 | A_13 |
| ATOM | 261 | CG2 | VAL | 31 | 75.829 | 54.587 | 14.377 | 1.00 | 10.00 | A_13 |
| ATOM | 262 | C | VAL | 31 | 79.208 | 53.040 | 13.216 | 1.00 | 20.29 | A_13 |
| ATOM | 263 | O | VAL | 31 | 79.330 | 51.814 | 13.282 | 1.00 | 14.02 | A_13 |
| ATOM | 264 | N | GLU | 32 | 79.913 | 53.790 | 12.370 | 1.00 | 23.94 | A_13 |
| ATOM | 266 | CA | GLU | 32 | 80.887 | 53.219 | 11.446 | 1.00 | 10.18 | A_13 |
| ATOM | 267 | CB | GLU | 32 | 81.406 | 54.285 | 10.502 | 1.00 | 16.50 | A_13 |
| ATOM | 268 | CG | GLU | 32 | 80.424 | 54.605 | 9.427 | 1.00 | 20.84 | A_13 |
| ATOM | 269 | CD | GLU | 32 | 80.330 | 56.080 | 9.155 | 1.00 | 22.31 | A_13 |
| ATOM | 270 | OE1 | GLU | 32 | 79.285 | 56.509 | 8.639 | 1.00 | 29.39 | A_13 |
| ATOM | 271 | OE2 | GLU | 32 | 81.294 | 56.812 | 9.458 | 1.00 | 22.01 | A_13 |
| ATOM | 272 | C | GLU | 32 | 82.056 | 52.565 | 12.137 | 1.00 | 18.93 | A_13 |
| ATOM | 273 | O | GLU | 32 | 82.474 | 51.470 | 11.753 | 1.00 | 24.42 | A_13 |
| ATOM | 274 | N | LYS | 33 | 82.610 | 53.241 | 13.139 | 1.00 | 19.78 | A_13 |
| ATOM | 276 | CA | LYS | 33 | 83.726 | 52.661 | 13.873 | 1.00 | 28.68 | A_13 |
| ATOM | 277 | CB | LYS | 33 | 84.340 | 53.681 | 14.837 | 1.00 | 18.54 | A_13 |
| ATOM | 278 | CG | LYS | 33 | 85.016 | 54.855 | 14.135 | 1.00 | 31.19 | A_13 |
| ATOM | 279 | CD | LYS | 33 | 86.135 | 54.425 | 13.148 | 1.00 | 40.31 | A_13 |
| ATOM | 280 | CE | LYS | 33 | 85.600 | 53.972 | 11.785 | 1.00 | 21.99 | A_13 |
| ATOM | 281 | NZ | LYS | 33 | 86.646 | 53.779 | 10.773 | 1.00 | 33.20 | A_13 |
| ATOM | 285 | C | LYS | 33 | 83.242 | 51.407 | 14.594 | 1.00 | 12.66 | A_13 |
| ATOM | 286 | O | LYS | 33 | 83.892 | 50.361 | 14.552 | 1.00 | 15.54 | A_13 |
| ATOM | 287 | N | ALA | 34 | 82.036 | 51.481 | 15.148 | 1.00 | 20.70 | A_13 |
| ATOM | 289 | CA | ALA | 34 | 81.453 | 50.344 | 15.843 | 1.00 | 10.00 | A_13 |

40/75

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 290 | CB | ALA | 34 | 80.040 | 50.651 | 16.279 | 1.00 | 18.59 | A_13 |
| ATOM | 291 | C | ALA | 34 | 81.468 | 49.119 | 14.940 | 1.00 | 13.45 | A_13 |
| ATOM | 292 | O | ALA | 34 | 82.067 | 48.095 | 15.284 | 1.00 | 15.90 | A_13 |
| ATOM | 293 | N | PHE | 35 | 80.857 | 49.234 | 13.766 | 1.00 | 19.57 | A_13 |
| ATOM | 295 | CA | PHE | 35 | 80.802 | 48.112 | 12.812 | 1.00 | 26.77 | A_13 |
| ATOM | 296 | CB | PHE | 35 | 79.837 | 48.423 | 11.660 | 1.00 | 17.34 | A_13 |
| ATOM | 297 | CG | PHE | 35 | 78.390 | 48.477 | 12.077 | 1.00 | 30.55 | A_13 |
| ATOM | 298 | CD1 | PHE | 35 | 77.838 | 47.464 | 12.863 | 1.00 | 26.58 | A_13 |
| ATOM | 299 | CD2 | PHE | 35 | 77.570 | 49.512 | 11.653 | 1.00 | 10.00 | A_13 |
| ATOM | 300 | CE1 | PHE | 35 | 76.494 | 47.485 | 13.212 | 1.00 | 12.45 | A_13 |
| ATOM | 301 | CE2 | PHE | 35 | 76.224 | 49.538 | 12.002 | 1.00 | 17.92 | A_13 |
| ATOM | 302 | CZ | PHE | 35 | 75.684 | 48.525 | 12.777 | 1.00 | 13.29 | A_13 |
| ATOM | 303 | C | PHE | 35 | 82.170 | 47.754 | 12.236 | 1.00 | 11.31 | A_13 |
| ATOM | 304 | O | PHE | 35 | 82.493 | 46.573 | 12.034 | 1.00 | 11.37 | A_13 |
| ATOM | 305 | N | LYS | 36 | 82.962 | 48.778 | 11.945 | 1.00 | 17.06 | A_13 |
| ATOM | 307 | CA | LYS | 36 | 84.293 | 48.573 | 11.400 | 1.00 | 17.41 | A_13 |
| ATOM | 308 | CB | LYS | 36 | 84.991 | 49.922 | 11.208 | 1.00 | 11.20 | A_13 |
| ATOM | 309 | CG | LYS | 36 | 86.282 | 49.792 | 10.439 | 1.00 | 28.84 | A_13 |
| ATOM | 310 | CD | LYS | 36 | 87.246 | 50.917 | 10.738 | 1.00 | 24.52 | A_13 |
| ATOM | 311 | CE | LYS | 36 | 88.542 | 50.703 | 9.978 | 1.00 | 12.87 | A_13 |
| ATOM | 312 | NZ | LYS | 36 | 88.264 | 50.536 | 8.514 | 1.00 | 23.69 | A_13 |
| ATOM | 316 | C | LYS | 36 | 85.122 | 47.685 | 12.345 | 1.00 | 16.09 | A_13 |
| ATOM | 317 | O | LYS | 36 | 85.701 | 46.686 | 11.938 | 1.00 | 21.50 | A_13 |
| ATOM | 318 | N | LYS | 37 | 85.173 | 48.057 | 13.613 | 1.00 | 12.42 | A_13 |
| ATOM | 320 | CA | LYS | 37 | 85.926 | 47.303 | 14.591 | 1.00 | 12.36 | A_13 |
| ATOM | 321 | CB | LYS | 37 | 85.953 | 48.066 | 15.917 | 1.00 | 13.65 | A_13 |
| ATOM | 322 | CG | LYS | 37 | 86.744 | 47.374 | 17.028 | 1.00 | 13.38 | A_13 |
| ATOM | 323 | CD | LYS | 37 | 88.192 | 47.125 | 16.616 | 1.00 | 38.32 | A_13 |
| ATOM | 324 | CE | LYS | 37 | 88.750 | 45.825 | 17.205 | 1.00 | 34.46 | A_13 |
| ATOM | 325 | NZ | LYS | 37 | 88.234 | 44.576 | 16.557 | 1.00 | 12.49 | A_13 |
| ATOM | 329 | C | LYS | 37 | 85.372 | 45.887 | 14.786 | 1.00 | 17.04 | A_13 |
| ATOM | 330 | O | LYS | 37 | 86.131 | 44.958 | 15.053 | 1.00 | 18.14 | A_13 |
| ATOM | 331 | N | ALA | 38 | 84.061 | 45.711 | 14.649 | 1.00 | 24.47 | A_13 |
| ATOM | 333 | CA | ALA | 38 | 83.452 | 44.392 | 14.822 | 1.00 | 11.03 | A_13 |
| ATOM | 334 | CB | ALA | 38 | 81.941 | 44.504 | 14.890 | 1.00 | 14.71 | A_13 |
| ATOM | 335 | C | ALA | 38 | 83.900 | 43.451 | 13.697 | 1.00 | 20.27 | A_13 |
| ATOM | 336 | O | ALA | 38 | 84.143 | 42.266 | 13.936 | 1.00 | 18.80 | A_13 |
| ATOM | 337 | N | PHE | 39 | 84.021 | 43.971 | 12.477 | 1.00 | 22.58 | A_13 |
| ATOM | 339 | CA | PHE | 39 | 84.492 | 43.158 | 11.355 | 1.00 | 18.87 | A_13 |
| ATOM | 340 | CB | PHE | 39 | 84.350 | 43.899 | 10.027 | 1.00 | 19.91 | A_13 |
| ATOM | 341 | CG | PHE | 39 | 82.993 | 43.783 | 9.414 | 1.00 | 10.00 | A_13 |
| ATOM | 342 | CD1 | PHE | 39 | 82.266 | 44.915 | 9.097 | 1.00 | 17.54 | A_13 |
| ATOM | 343 | CD2 | PHE | 39 | 82.438 | 42.533 | 9.143 | 1.00 | 15.92 | A_13 |
| ATOM | 344 | CE1 | PHE | 39 | 81.008 | 44.808 | 8.520 | 1.00 | 20.75 | A_13 |
| ATOM | 345 | CE2 | PHE | 39 | 81.186 | 42.418 | 8.569 | 1.00 | 10.00 | A_13 |
| ATOM | 346 | CZ | PHE | 39 | 80.467 | 43.555 | 8.252 | 1.00 | 10.00 | A_13 |
| ATOM | 347 | C | PHE | 39 | 85.955 | 42.827 | 11.589 | 1.00 | 16.52 | A_13 |
| ATOM | 348 | O | PHE | 39 | 86.382 | 41.689 | 11.387 | 1.00 | 19.70 | A_13 |
| ATOM | 349 | N | LYS | 40 | 86.699 | 43.822 | 12.072 | 1.00 | 21.31 | A_13 |
| ATOM | 351 | CA | LYS | 40 | 88.117 | 43.673 | 12.369 | 1.00 | 20.07 | A_13 |
| ATOM | 352 | CB | LYS | 40 | 88.703 | 44.967 | 12.927 | 1.00 | 13.77 | A_13 |
| ATOM | 353 | CG | LYS | 40 | 90.192 | 44.885 | 13.171 | 1.00 | 11.54 | A_13 |
| ATOM | 354 | CD | LYS | 40 | 90.757 | 46.242 | 13.507 | 1.00 | 10.34 | A_13 |
| ATOM | 355 | CE | LYS | 40 | 92.236 | 46.142 | 13.838 | 1.00 | 11.24 | A_13 |
| ATOM | 356 | NZ | LYS | 40 | 92.468 | 45.518 | 15.179 | 1.00 | 27.33 | A_13 |
| ATOM | 360 | C | LYS | 40 | 88.352 | 42.534 | 13.337 | 1.00 | 12.06 | A_13 |
| ATOM | 361 | O | LYS | 40 | 89.252 | 41.719 | 13.124 | 1.00 | 25.09 | A_13 |
| ATOM | 362 | N | VAL | 41 | 87.495 | 42.418 | 14.349 | 1.00 | 12.26 | A_13 |
| ATOM | 364 | CA | VAL | 41 | 87.630 | 41.331 | 15.325 | 1.00 | 17.89 | A_13 |
| ATOM | 365 | CB | VAL | 41 | 86.351 | 41.205 | 16.216 | 1.00 | 10.00 | A_13 |
| ATOM | 366 | CG1 | VAL | 41 | 86.298 | 39.865 | 16.894 | 1.00 | 23.82 | A_13 |
| ATOM | 367 | CG2 | VAL | 41 | 86.329 | 42.274 | 17.259 | 1.00 | 17.65 | A_13 |
| ATOM | 368 | C | VAL | 41 | 87.822 | 40.009 | 14.560 | 1.00 | 23.06 | A_13 |
| ATOM | 369 | O | VAL | 41 | 88.664 | 39.168 | 14.912 | 1.00 | 11.82 | A_13 |
| ATOM | 370 | N | TRP | 42 | 87.069 | 39.871 | 13.471 | 1.00 | 21.42 | A_13 |
| ATOM | 372 | CA | TRP | 42 | 87.085 | 38.666 | 12.661 | 1.00 | 21.32 | A_13 |
| ATOM | 373 | CB | TRP | 42 | 85.713 | 38.476 | 12.009 | 1.00 | 18.84 | A_13 |
| ATOM | 374 | CG | TRP | 42 | 84.605 | 38.387 | 13.025 | 1.00 | 25.92 | A_13 |
| ATOM | 375 | CD2 | TRP | 42 | 84.437 | 37.369 | 14.024 | 1.00 | 16.65 | A_13 |
| ATOM | 376 | CE2 | TRP | 42 | 83.260 | 37.680 | 14.737 | 1.00 | 17.58 | A_13 |
| ATOM | 377 | CE3 | TRP | 42 | 85.165 | 36.223 | 14.380 | 1.00 | 11.14 | A_13 |
| ATOM | 378 | CD1 | TRP | 42 | 83.563 | 39.249 | 13.179 | 1.00 | 10.00 | A_13 |
| ATOM | 379 | NE1 | TRP | 42 | 82.755 | 38.832 | 14.200 | 1.00 | 10.91 | A_13 |
| ATOM | 381 | CZ2 | TRP | 42 | 82.785 | 36.879 | 15.793 | 1.00 | 14.81 | A_13 |
| ATOM | 382 | CZ3 | TRP | 42 | 84.691 | 35.425 | 15.436 | 1.00 | 23.68 | A_13 |
| ATOM | 383 | CH2 | TRP | 42 | 83.513 | 35.759 | 16.125 | 1.00 | 12.75 | A_13 |
| ATOM | 384 | C | TRP | 42 | 88.190 | 38.600 | 11.623 | 1.00 | 27.45 | A_13 |

41/75

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 385 | O | TRP | 42 | 88.834 | 37.556 | 11.472 | 1.00 | 11.84 | A_13 |
| ATOM | 386 | N | SER | 43 | 88.413 | 39.702 | 10.909 | 1.00 | 25.46 | A_13 |
| ATOM | 388 | CA | SER | 43 | 89.449 | 39.740 | 9.881 | 1.00 | 19.61 | A_13 |
| ATOM | 389 | CB | SER | 43 | 89.342 | 40.993 | 8.991 | 1.00 | 16.16 | A_13 |
| ATOM | 390 | OG | SER | 43 | 89.495 | 42.199 | 9.709 | 1.00 | 26.34 | A_13 |
| ATOM | 392 | C | SER | 43 | 90.837 | 39.615 | 10.491 | 1.00 | 11.53 | A_13 |
| ATOM | 393 | O | SER | 43 | 91.758 | 39.119 | 9.834 | 1.00 | 17.99 | A_13 |
| ATOM | 394 | N | ASP | 44 | 90.949 | 39.973 | 11.771 | 1.00 | 10.00 | A_13 |
| ATOM | 396 | CA | ASP | 44 | 92.206 | 39.908 | 12.505 | 1.00 | 16.90 | A_13 |
| ATOM | 397 | CB | ASP | 44 | 92.057 | 40.588 | 13.857 | 1.00 | 17.79 | A_13 |
| ATOM | 398 | CG | ASP | 44 | 92.544 | 42.013 | 13.839 | 1.00 | 15.93 | A_13 |
| ATOM | 399 | OD1 | ASP | 44 | 92.605 | 42.618 | 14.920 | 1.00 | 17.21 | A_13 |
| ATOM | 400 | OD2 | ASP | 44 | 92.874 | 42.533 | 12.754 | 1.00 | 19.50 | A_13 |
| ATOM | 401 | C | ASP | 44 | 92.781 | 38.523 | 12.729 | 1.00 | 26.12 | A_13 |
| ATOM | 402 | O | ASP | 44 | 93.996 | 38.362 | 12.897 | 1.00 | 21.21 | A_13 |
| ATOM | 403 | N | VAL | 45 | 91.911 | 37.523 | 12.745 | 1.00 | 20.89 | A_13 |
| ATOM | 405 | CA | VAL | 45 | 92.353 | 36.161 | 12.996 | 1.00 | 27.53 | A_13 |
| ATOM | 406 | CB | VAL | 45 | 91.853 | 35.678 | 14.381 | 1.00 | 16.30 | A_13 |
| ATOM | 407 | CG1 | VAL | 45 | 92.557 | 36.472 | 15.504 | 1.00 | 10.00 | A_13 |
| ATOM | 408 | CG2 | VAL | 45 | 90.348 | 35.857 | 14.495 | 1.00 | 10.86 | A_13 |
| ATOM | 409 | C | VAL | 45 | 91.928 | 35.187 | 11.911 | 1.00 | 24.33 | A_13 |
| ATOM | 410 | O | VAL | 45 | 91.864 | 33.978 | 12.157 | 1.00 | 18.84 | A_13 |
| ATOM | 411 | N | THR | 46 | 91.750 | 35.705 | 10.694 | 1.00 | 16.30 | A_13 |
| ATOM | 413 | CA | THR | 46 | 91.293 | 34.893 | 9.574 | 1.00 | 14.48 | A_13 |
| ATOM | 414 | CB | THR | 46 | 89.750 | 34.796 | 9.662 | 1.00 | 22.05 | A_13 |
| ATOM | 415 | OG1 | THR | 46 | 89.279 | 33.609 | 9.028 | 1.00 | 31.53 | A_13 |
| ATOM | 417 | CG2 | THR | 46 | 89.112 | 36.014 | 9.040 | 1.00 | 10.99 | A_13 |
| ATOM | 418 | C | THR | 46 | 91.716 | 35.575 | 8.257 | 1.00 | 25.10 | A_13 |
| ATOM | 419 | O | THR | 46 | 92.022 | 36.764 | 8.256 | 1.00 | 17.64 | A_13 |
| ATOM | 420 | N | PRO | 47 | 91.688 | 34.845 | 7.114 | 1.00 | 15.31 | A_13 |
| ATOM | 421 | CD | PRO | 47 | 91.459 | 33.398 | 6.985 | 1.00 | 17.94 | A_13 |
| ATOM | 422 | CA | PRO | 47 | 92.069 | 35.416 | 5.815 | 1.00 | 21.50 | A_13 |
| ATOM | 423 | CB | PRO | 47 | 92.199 | 34.182 | 4.911 | 1.00 | 17.57 | A_13 |
| ATOM | 424 | CG | PRO | 47 | 92.369 | 33.041 | 5.848 | 1.00 | 27.45 | A_13 |
| ATOM | 425 | C | PRO | 47 | 90.991 | 36.348 | 5.256 | 1.00 | 21.44 | A_13 |
| ATOM | 426 | O | PRO | 47 | 91.095 | 36.788 | 4.116 | 1.00 | 11.08 | A_13 |
| ATOM | 427 | N | LEU | 48 | 89.918 | 36.567 | 6.018 | 1.00 | 10.00 | A_13 |
| ATOM | 429 | CA | LEU | 48 | 88.826 | 37.434 | 5.581 | 1.00 | 22.09 | A_13 |
| ATOM | 430 | CB | LEU | 48 | 87.575 | 37.212 | 6.432 | 1.00 | 15.92 | A_13 |
| ATOM | 431 | CG | LEU | 48 | 86.848 | 35.867 | 6.435 | 1.00 | 13.58 | A_13 |
| ATOM | 432 | CD1 | LEU | 48 | 85.931 | 35.811 | 7.654 | 1.00 | 25.90 | A_13 |
| ATOM | 433 | CD2 | LEU | 48 | 86.073 | 35.666 | 5.157 | 1.00 | 16.47 | A_13 |
| ATOM | 434 | C | LEU | 48 | 89.156 | 38.916 | 5.641 | 1.00 | 21.20 | A_13 |
| ATOM | 435 | O | LEU | 48 | 89.936 | 39.366 | 6.480 | 1.00 | 17.28 | A_13 |
| ATOM | 436 | N | ASN | 49 | 88.569 | 39.670 | 4.723 | 1.00 | 26.12 | A_13 |
| ATOM | 438 | CA | ASN | 49 | 88.738 | 41.112 | 4.717 | 1.00 | 26.84 | A_13 |
| ATOM | 439 | CB | ASN | 49 | 89.936 | 41.569 | 3.885 | 1.00 | 18.29 | A_13 |
| ATOM | 440 | CG | ASN | 49 | 90.010 | 40.912 | 2.568 | 1.00 | 22.55 | A_13 |
| ATOM | 441 | OD1 | ASN | 49 | 90.928 | 40.131 | 2.305 | 1.00 | 24.41 | A_13 |
| ATOM | 442 | ND2 | ASN | 49 | 89.068 | 41.235 | 1.693 | 1.00 | 46.51 | A_13 |
| ATOM | 445 | C | ASN | 49 | 87.416 | 41.705 | 4.259 | 1.00 | 12.18 | A_13 |
| ATOM | 446 | O | ASN | 49 | 86.732 | 41.128 | 3.400 | 1.00 | 20.77 | A_13 |
| ATOM | 447 | N | PHE | 50 | 87.025 | 42.802 | 4.900 | 1.00 | 21.39 | A_13 |
| ATOM | 449 | CA | PHE | 50 | 85.738 | 43.439 | 4.642 | 1.00 | 10.00 | A_13 |
| ATOM | 450 | CB | PHE | 50 | 84.914 | 43.440 | 5.932 | 1.00 | 11.45 | A_13 |
| ATOM | 451 | CG | PHE | 50 | 84.863 | 42.098 | 6.629 | 1.00 | 10.63 | A_13 |
| ATOM | 452 | CD1 | PHE | 50 | 85.886 | 41.705 | 7.490 | 1.00 | 10.00 | A_13 |
| ATOM | 453 | CD2 | PHE | 50 | 83.809 | 41.216 | 6.395 | 1.00 | 14.63 | A_13 |
| ATOM | 454 | CE1 | PHE | 50 | 85.858 | 40.457 | 8.097 | 1.00 | 26.88 | A_13 |
| ATOM | 455 | CE2 | PHE | 50 | 83.773 | 39.963 | 7.000 | 1.00 | 21.13 | A_13 |
| ATOM | 456 | CZ | PHE | 50 | 84.801 | 39.581 | 7.852 | 1.00 | 10.30 | A_13 |
| ATOM | 457 | C | PHE | 50 | 85.867 | 44.842 | 4.093 | 1.00 | 22.56 | A_13 |
| ATOM | 458 | O | PHE | 50 | 86.638 | 45.644 | 4.612 | 1.00 | 19.33 | A_13 |
| ATOM | 459 | N | THR | 51 | 85.099 | 45.129 | 3.044 | 1.00 | 21.47 | A_13 |
| ATOM | 461 | CA | THR | 51 | 85.125 | 46.433 | 2.371 | 1.00 | 24.21 | A_13 |
| ATOM | 462 | CB | THR | 51 | 85.602 | 46.306 | 0.895 | 1.00 | 15.39 | A_13 |
| ATOM | 463 | OG1 | THR | 51 | 86.950 | 45.811 | 0.853 | 1.00 | 24.33 | A_13 |
| ATOM | 465 | CG2 | THR | 51 | 85.551 | 47.654 | 0.192 | 1.00 | 25.47 | A_13 |
| ATOM | 466 | C | THR | 51 | 83.735 | 47.048 | 2.359 | 1.00 | 22.17 | A_13 |
| ATOM | 467 | O | THR | 51 | 82.766 | 46.421 | 1.912 | 1.00 | 20.53 | A_13 |
| ATOM | 468 | N | ARG | 52 | 83.653 | 48.294 | 2.797 | 1.00 | 16.53 | A_13 |
| ATOM | 470 | CA | ARG | 52 | 82.393 | 49.004 | 2.871 | 1.00 | 10.00 | A_13 |
| ATOM | 471 | CB | ARG | 52 | 82.490 | 50.085 | 3.939 | 1.00 | 10.00 | A_13 |
| ATOM | 472 | CG | ARG | 52 | 81.201 | 50.778 | 4.259 | 1.00 | 12.47 | A_13 |
| ATOM | 473 | CD | ARG | 52 | 81.462 | 51.879 | 5.278 | 1.00 | 19.61 | A_13 |
| ATOM | 474 | NE | ARG | 52 | 80.371 | 52.836 | 5.333 | 1.00 | 30.55 | A_13 |
| ATOM | 476 | CZ | ARG | 52 | 80.489 | 54.074 | 5.795 | 1.00 | 24.06 | A_13 |

42/75

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 477 | NH1 | ARG | 52 | 81.661 | 54.508 | 6.257 | 1.00 | 21.24 | A_13 |
| ATOM | 480 | NH2 | ARG | 52 | 79.421 | 54.862 | 5.829 | 1.00 | 27.78 | A_13 |
| ATOM | 483 | C | ARG | 52 | 81.980 | 49.620 | 1.540 | 1.00 | 30.22 | A_13 |
| ATOM | 484 | O | ARG | 52 | 82.782 | 50.269 | 0.859 | 1.00 | 16.27 | A_13 |
| ATOM | 485 | N | LEU | 53 | 80.730 | 49.372 | 1.161 | 1.00 | 21.07 | A_13 |
| ATOM | 487 | CA | LEU | 53 | 80.159 | 49.914 | -0.062 | 1.00 | 15.73 | A_13 |
| ATOM | 488 | CB | LEU | 53 | 79.435 | 48.831 | -0.868 | 1.00 | 11.53 | A_13 |
| ATOM | 489 | CG | LEU | 53 | 80.304 | 47.770 | -1.530 | 1.00 | 10.00 | A_13 |
| ATOM | 490 | CD1 | LEU | 53 | 79.429 | 46.790 | -2.296 | 1.00 | 13.21 | A_13 |
| ATOM | 491 | CD2 | LEU | 53 | 81.280 | 48.443 | -2.448 | 1.00 | 12.78 | A_13 |
| ATOM | 492 | C | LEU | 53 | 79.149 | 50.932 | 0.421 | 1.00 | 10.00 | A_13 |
| ATOM | 493 | O | LEU | 53 | 78.463 | 50.713 | 1.411 | 1.00 | 13.62 | A_13 |
| ATOM | 494 | N | HIS | 54 | 79.043 | 52.041 | -0.283 | 1.00 | 15.73 | A_13 |
| ATOM | 496 | CA | HIS | 54 | 78.102 | 53.065 | 0.126 | 1.00 | 12.47 | A_13 |
| ATOM | 497 | CB | HIS | 54 | 78.765 | 54.435 | 0.011 | 1.00 | 15.18 | A_13 |
| ATOM | 498 | CG | HIS | 54 | 79.967 | 54.589 | 0.884 | 1.00 | 21.27 | A_13 |
| ATOM | 499 | CD2 | HIS | 54 | 81.207 | 54.056 | 0.798 | 1.00 | 25.30 | A_13 |
| ATOM | 500 | ND1 | HIS | 54 | 79.951 | 55.338 | 2.043 | 1.00 | 16.48 | A_13 |
| ATOM | 502 | CE1 | HIS | 54 | 81.127 | 55.255 | 2.633 | 1.00 | 21.62 | A_13 |
| ATOM | 503 | NE2 | HIS | 54 | 81.910 | 54.482 | 1.899 | 1.00 | 29.91 | A_13 |
| ATOM | 505 | C | HIS | 54 | 76.796 | 53.044 | -0.664 | 1.00 | 15.50 | A_13 |
| ATOM | 506 | O | HIS | 54 | 75.914 | 53.849 | -0.403 | 1.00 | 21.80 | A_13 |
| ATOM | 507 | N | ASP | 55 | 76.707 | 52.178 | -1.671 | 1.00 | 18.31 | A_13 |
| ATOM | 509 | CA | ASP | 55 | 75.509 | 52.077 | -2.502 | 1.00 | 17.23 | A_13 |
| ATOM | 510 | CB | ASP | 55 | 75.645 | 52.928 | -3.773 | 1.00 | 19.94 | A_13 |
| ATOM | 511 | CG | ASP | 55 | 75.864 | 54.393 | -3.495 | 1.00 | 26.81 | A_13 |
| ATOM | 512 | OD1 | ASP | 55 | 75.059 | 54.991 | -2.741 | 1.00 | 35.97 | A_13 |
| ATOM | 513 | OD2 | ASP | 55 | 76.839 | 54.948 | -4.058 | 1.00 | 25.09 | A_13 |
| ATOM | 514 | C | ASP | 55 | 75.343 | 50.645 | -2.970 | 1.00 | 21.50 | A_13 |
| ATOM | 515 | O | ASP | 55 | 76.286 | 49.862 | -2.929 | 1.00 | 17.45 | A_13 |
| ATOM | 516 | N | GLY | 56 | 74.160 | 50.337 | -3.489 | 1.00 | 10.31 | A_13 |
| ATOM | 518 | CA | GLY | 56 | 73.897 | 49.014 | -4.014 | 1.00 | 13.67 | A_13 |
| ATOM | 519 | C | GLY | 56 | 73.842 | 47.869 | -3.030 | 1.00 | 17.61 | A_13 |
| ATOM | 520 | O | GLY | 56 | 73.683 | 48.065 | -1.825 | 1.00 | 12.57 | A_13 |
| ATOM | 521 | N | ILE | 57 | 73.943 | 46.653 | -3.560 | 1.00 | 22.27 | A_13 |
| ATOM | 523 | CA | ILE | 57 | 73.895 | 45.460 | -2.737 | 1.00 | 11.39 | A_13 |
| ATOM | 524 | CB | ILE | 57 | 72.941 | 44.391 | -3.347 | 1.00 | 22.87 | A_13 |
| ATOM | 525 | CG2 | ILE | 57 | 73.365 | 42.995 | -2.955 | 1.00 | 22.98 | A_13 |
| ATOM | 526 | CG1 | ILE | 57 | 71.522 | 44.582 | -2.787 | 1.00 | 30.87 | A_13 |
| ATOM | 527 | CD1 | ILE | 57 | 71.002 | 46.022 | -2.796 | 1.00 | 28.15 | A_13 |
| ATOM | 528 | C | ILE | 57 | 75.289 | 44.919 | -2.446 | 1.00 | 22.32 | A_13 |
| ATOM | 529 | O | ILE | 57 | 76.140 | 44.849 | -3.332 | 1.00 | 25.00 | A_13 |
| ATOM | 530 | N | ALA | 58 | 75.517 | 44.631 | -1.168 | 1.00 | 25.02 | A_13 |
| ATOM | 532 | CA | ALA | 58 | 76.773 | 44.105 | -0.669 | 1.00 | 15.45 | A_13 |
| ATOM | 533 | CB | ALA | 58 | 77.366 | 45.060 | 0.358 | 1.00 | 11.62 | A_13 |
| ATOM | 534 | C | ALA | 58 | 76.438 | 42.780 | -0.006 | 1.00 | 12.08 | A_13 |
| ATOM | 535 | O | ALA | 58 | 75.289 | 42.521 | 0.307 | 1.00 | 13.30 | A_13 |
| ATOM | 536 | N | ASP | 59 | 77.449 | 41.968 | 0.247 | 1.00 | 14.79 | A_13 |
| ATOM | 538 | CA | ASP | 59 | 77.245 | 40.675 | 0.880 | 1.00 | 18.50 | A_13 |
| ATOM | 539 | CB | ASP | 59 | 78.608 | 39.974 | 1.093 | 1.00 | 10.83 | A_13 |
| ATOM | 540 | CG | ASP | 59 | 79.425 | 39.858 | -0.210 | 1.00 | 23.35 | A_13 |
| ATOM | 541 | OD1 | ASP | 59 | 80.598 | 40.266 | -0.236 | 1.00 | 17.98 | A_13 |
| ATOM | 542 | OD2 | ASP | 59 | 78.896 | 39.379 | -1.230 | 1.00 | 16.89 | A_13 |
| ATOM | 543 | C | ASP | 59 | 76.480 | 40.806 | 2.200 | 1.00 | 13.69 | A_13 |
| ATOM | 544 | O | ASP | 59 | 75.402 | 40.227 | 2.380 | 1.00 | 15.93 | A_13 |
| ATOM | 545 | N | ILE | 60 | 77.025 | 41.596 | 3.109 | 1.00 | 13.15 | A_13 |
| ATOM | 547 | CA | ILE | 60 | 76.422 | 41.800 | 4.412 | 1.00 | 12.20 | A_13 |
| ATOM | 548 | CB | ILE | 60 | 77.500 | 41.695 | 5.508 | 1.00 | 12.12 | A_13 |
| ATOM | 549 | CG2 | ILE | 60 | 76.921 | 42.060 | 6.864 | 1.00 | 19.27 | A_13 |
| ATOM | 550 | CG1 | ILE | 60 | 78.118 | 40.287 | 5.481 | 1.00 | 10.00 | A_13 |
| ATOM | 551 | CD1 | ILE | 60 | 79.330 | 40.120 | 6.360 | 1.00 | 10.00 | A_13 |
| ATOM | 552 | C | ILE | 60 | 75.743 | 43.164 | 4.456 | 1.00 | 17.78 | A_13 |
| ATOM | 553 | O | ILE | 60 | 76.410 | 44.193 | 4.478 | 1.00 | 18.65 | A_13 |
| ATOM | 554 | N | MET | 61 | 74.416 | 43.168 | 4.431 | 1.00 | 12.54 | A_13 |
| ATOM | 556 | CA | MET | 61 | 73.640 | 44.416 | 4.476 | 1.00 | 12.86 | A_13 |
| ATOM | 557 | CB | MET | 61 | 72.385 | 44.314 | 3.604 | 1.00 | 18.16 | A_13 |
| ATOM | 558 | CG | MET | 61 | 72.634 | 43.979 | 2.141 | 1.00 | 10.00 | A_13 |
| ATOM | 559 | SD | MET | 61 | 73.374 | 45.314 | 1.251 | 1.00 | 10.69 | A_13 |
| ATOM | 560 | CE | MET | 61 | 71.836 | 46.299 | 0.764 | 1.00 | 10.00 | A_13 |
| ATOM | 561 | C | MET | 61 | 73.239 | 44.666 | 5.921 | 1.00 | 10.15 | A_13 |
| ATOM | 562 | O | MET | 61 | 72.584 | 43.838 | 6.547 | 1.00 | 18.13 | A_13 |
| ATOM | 563 | N | ILE | 62 | 73.706 | 45.784 | 6.456 | 1.00 | 15.60 | A_13 |
| ATOM | 565 | CA | ILE | 62 | 73.452 | 46.170 | 7.837 | 1.00 | 18.55 | A_13 |
| ATOM | 566 | CB | ILE | 62 | 74.723 | 46.828 | 8.437 | 1.00 | 10.00 | A_13 |
| ATOM | 567 | CG2 | ILE | 62 | 74.498 | 47.163 | 9.900 | 1.00 | 26.36 | A_13 |
| ATOM | 568 | CG1 | ILE | 62 | 75.936 | 45.897 | 8.302 | 1.00 | 11.04 | A_13 |
| ATOM | 569 | CD1 | ILE | 62 | 77.228 | 46.481 | 8.891 | 1.00 | 10.00 | A_13 |

43/75

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 570 | C | ILE | 62 | 72.289 | 47.172 | 7.920 | 1.00 | 17.99 | A_13 |
| ATOM | 571 | O | ILE | 62 | 72.335 | 48.208 | 7.264 | 1.00 | 12.72 | A_13 |
| ATOM | 572 | N | SER | 63 | 71.285 | 46.896 | 8.751 | 1.00 | 10.00 | A_13 |
| ATOM | 574 | CA | SER | 63 | 70.149 | 47.803 | 8.882 | 1.00 | 12.52 | A_13 |
| ATOM | 575 | CB | SER | 63 | 69.016 | 47.364 | 7.956 | 1.00 | 13.06 | A_13 |
| ATOM | 576 | OG | SER | 63 | 68.448 | 46.146 | 8.415 | 1.00 | 27.90 | A_13 |
| ATOM | 578 | C | SER | 63 | 69.625 | 47.854 | 10.314 | 1.00 | 13.14 | A_13 |
| ATOM | 579 | O | SER | 63 | 69.869 | 46.951 | 11.101 | 1.00 | 22.10 | A_13 |
| ATOM | 580 | N | PHE | 64 | 68.919 | 48.932 | 10.640 | 1.00 | 21.17 | A_13 |
| ATOM | 582 | CA | PHE | 64 | 68.317 | 49.139 | 11.954 | 1.00 | 22.01 | A_13 |
| ATOM | 583 | CB | PHE | 64 | 68.777 | 50.468 | 12.574 | 1.00 | 10.98 | A_13 |
| ATOM | 584 | CG | PHE | 64 | 70.189 | 50.448 | 13.092 | 1.00 | 10.00 | A_13 |
| ATOM | 585 | CD1 | PHE | 64 | 70.473 | 49.885 | 14.322 | 1.00 | 10.00 | A_13 |
| ATOM | 586 | CD2 | PHE | 64 | 71.229 | 51.016 | 12.357 | 1.00 | 16.56 | A_13 |
| ATOM | 587 | CE1 | PHE | 64 | 71.777 | 49.885 | 14.825 | 1.00 | 10.00 | A_13 |
| ATOM | 588 | CE2 | PHE | 64 | 72.540 | 51.025 | 12.846 | 1.00 | 10.00 | A_13 |
| ATOM | 589 | CZ | PHE | 64 | 72.812 | 50.459 | 14.081 | 1.00 | 18.83 | A_13 |
| ATOM | 590 | C | PHE | 64 | 66.825 | 49.207 | 11.675 | 1.00 | 22.55 | A_13 |
| ATOM | 591 | O | PHE | 64 | 66.405 | 49.940 | 10.779 | 1.00 | 19.49 | A_13 |
| ATOM | 592 | N | GLY | 65 | 66.031 | 48.485 | 12.453 | 1.00 | 13.69 | A_13 |
| ATOM | 594 | CA | GLY | 65 | 64.593 | 48.491 | 12.238 | 1.00 | 10.70 | A_13 |
| ATOM | 595 | C | GLY | 65 | 63.894 | 48.138 | 13.521 | 1.00 | 12.62 | A_13 |
| ATOM | 596 | O | GLY | 65 | 64.559 | 47.777 | 14.491 | 1.00 | 18.29 | A_13 |
| ATOM | 597 | N | ILE | 66 | 62.577 | 48.309 | 13.565 | 1.00 | 13.69 | A_13 |
| ATOM | 599 | CA | ILE | 66 | 61.803 | 47.968 | 14.760 | 1.00 | 21.58 | A_13 |
| ATOM | 600 | CB | ILE | 66 | 61.227 | 49.228 | 15.503 | 1.00 | 30.51 | A_13 |
| ATOM | 601 | CG2 | ILE | 66 | 62.351 | 50.110 | 16.025 | 1.00 | 10.43 | A_13 |
| ATOM | 602 | CG1 | ILE | 66 | 60.332 | 50.062 | 14.586 | 1.00 | 14.56 | A_13 |
| ATOM | 603 | CD1 | ILE | 66 | 59.587 | 51.149 | 15.333 | 1.00 | 16.94 | A_13 |
| ATOM | 604 | C | ILE | 66 | 60.662 | 47.030 | 14.361 | 1.00 | 10.81 | A_13 |
| ATOM | 605 | O | ILE | 66 | 60.311 | 46.962 | 13.188 | 1.00 | 10.00 | A_13 |
| ATOM | 606 | N | LYS | 67 | 60.143 | 46.271 | 15.330 | 1.00 | 10.00 | A_13 |
| ATOM | 608 | CA | LYS | 67 | 59.036 | 45.327 | 15.103 | 1.00 | 10.23 | A_13 |
| ATOM | 609 | CB | LYS | 67 | 57.689 | 46.042 | 15.268 | 1.00 | 10.29 | A_13 |
| ATOM | 610 | CG | LYS | 67 | 57.584 | 46.895 | 16.510 | 1.00 | 14.63 | A_13 |
| ATOM | 611 | CD | LYS | 67 | 57.646 | 46.056 | 17.774 | 1.00 | 14.94 | A_13 |
| ATOM | 612 | CE | LYS | 67 | 57.382 | 46.923 | 18.986 | 1.00 | 22.99 | A_13 |
| ATOM | 613 | NZ | LYS | 67 | 57.480 | 46.174 | 20.258 | 1.00 | 28.27 | A_13 |
| ATOM | 617 | C | LYS | 67 | 59.113 | 44.633 | 13.726 | 1.00 | 17.91 | A_13 |
| ATOM | 618 | O | LYS | 67 | 60.167 | 44.106 | 13.366 | 1.00 | 24.16 | A_13 |
| ATOM | 619 | N | GLU | 68 | 58.027 | 44.690 | 12.949 | 1.00 | 12.72 | A_13 |
| ATOM | 621 | CA | GLU | 68 | 57.960 | 44.067 | 11.624 | 1.00 | 16.06 | A_13 |
| ATOM | 622 | CB | GLU | 68 | 56.505 | 44.019 | 11.128 | 1.00 | 26.89 | A_13 |
| ATOM | 623 | CG | GLU | 68 | 55.566 | 43.258 | 12.087 | 1.00 | 36.97 | A_13 |
| ATOM | 624 | CD | GLU | 68 | 54.217 | 43.973 | 12.381 | 1.00 | 41.61 | A_13 |
| ATOM | 625 | OE1 | GLU | 68 | 53.289 | 43.921 | 11.537 | 1.00 | 17.31 | A_13 |
| ATOM | 626 | OE2 | GLU | 68 | 54.074 | 44.561 | 13.485 | 1.00 | 26.72 | A_13 |
| ATOM | 627 | C | GLU | 68 | 58.823 | 44.911 | 10.705 | 1.00 | 22.50 | A_13 |
| ATOM | 628 | O | GLU | 68 | 58.587 | 46.093 | 10.532 | 1.00 | 20.64 | A_13 |
| ATOM | 629 | N | HIS | 69 | 59.848 | 44.315 | 10.120 | 1.00 | 16.43 | A_13 |
| ATOM | 631 | CA | HIS | 69 | 60.732 | 45.102 | 9.283 | 1.00 | 13.69 | A_13 |
| ATOM | 632 | CB | HIS | 69 | 61.930 | 45.603 | 10.103 | 1.00 | 10.97 | A_13 |
| ATOM | 633 | CG | HIS | 69 | 62.786 | 44.502 | 10.643 | 1.00 | 24.02 | A_13 |
| ATOM | 634 | CD2 | HIS | 69 | 63.873 | 43.876 | 10.133 | 1.00 | 10.00 | A_13 |
| ATOM | 635 | ND1 | HIS | 69 | 62.512 | 43.876 | 11.839 | 1.00 | 17.68 | A_13 |
| ATOM | 637 | CE1 | HIS | 69 | 63.384 | 42.912 | 12.041 | 1.00 | 12.53 | A_13 |
| ATOM | 638 | NE2 | HIS | 69 | 64.228 | 42.888 | 11.020 | 1.00 | 10.00 | A_13 |
| ATOM | 639 | C | HIS | 69 | 61.214 | 44.469 | 7.983 | 1.00 | 21.28 | A_13 |
| ATOM | 640 | O | HIS | 69 | 62.314 | 44.780 | 7.529 | 1.00 | 18.74 | A_13 |
| ATOM | 641 | N | GLY | 70 | 60.451 | 43.537 | 7.411 | 1.00 | 13.11 | A_13 |
| ATOM | 643 | CA | GLY | 70 | 60.832 | 42.968 | 6.127 | 1.00 | 10.00 | A_13 |
| ATOM | 644 | C | GLY | 70 | 61.262 | 41.533 | 5.936 | 1.00 | 10.00 | A_13 |
| ATOM | 645 | O | GLY | 70 | 61.523 | 41.125 | 4.794 | 1.00 | 15.12 | A_13 |
| ATOM | 646 | N | ASP | 71 | 61.412 | 40.768 | 7.012 | 1.00 | 19.99 | A_13 |
| ATOM | 648 | CA | ASP | 71 | 61.842 | 39.381 | 6.862 | 1.00 | 19.99 | A_13 |
| ATOM | 649 | CB | ASP | 71 | 63.332 | 39.223 | 7.218 | 1.00 | 10.00 | A_13 |
| ATOM | 650 | CG | ASP | 71 | 63.672 | 39.752 | 8.592 | 1.00 | 23.52 | A_13 |
| ATOM | 651 | OD1 | ASP | 71 | 64.846 | 40.110 | 8.803 | 1.00 | 13.38 | A_13 |
| ATOM | 652 | OD2 | ASP | 71 | 62.774 | 39.812 | 9.464 | 1.00 | 12.94 | A_13 |
| ATOM | 653 | C | ASP | 71 | 60.998 | 38.377 | 7.632 | 1.00 | 22.07 | A_13 |
| ATOM | 654 | O | ASP | 71 | 61.319 | 37.190 | 7.649 | 1.00 | 24.45 | A_13 |
| ATOM | 655 | N | PHE | 72 | 59.946 | 38.865 | 8.292 | 1.00 | 14.15 | A_13 |
| ATOM | 657 | CA | PHE | 72 | 59.040 | 38.035 | 9.094 | 1.00 | 10.00 | A_13 |
| ATOM | 658 | CB | PHE | 72 | 58.410 | 36.905 | 8.272 | 1.00 | 10.00 | A_13 |
| ATOM | 659 | CG | PHE | 72 | 57.360 | 37.387 | 7.332 | 1.00 | 10.00 | A_13 |
| ATOM | 660 | CD1 | PHE | 72 | 56.115 | 37.773 | 7.815 | 1.00 | 23.01 | A_13 |
| ATOM | 661 | CD2 | PHE | 72 | 57.624 | 37.507 | 5.973 | 1.00 | 12.52 | A_13 |

44/75

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 662 | CE1 | PHE | 72 | 55.144 | 38.290 | 6.950 | 1.00 | 18.99 | A_13 |
| ATOM | 663 | CE2 | PHE | 72 | 56.662 | 38.023 | 5.091 | 1.00 | 13.37 | A_13 |
| ATOM | 664 | CZ | PHE | 72 | 55.420 | 38.413 | 5.576 | 1.00 | 22.50 | A_13 |
| ATOM | 665 | C | PHE | 72 | 59.634 | 37.523 | 10.392 | 1.00 | 16.31 | A_13 |
| ATOM | 666 | O | PHE | 72 | 59.111 | 36.596 | 11.021 | 1.00 | 15.64 | A_13 |
| ATOM | 667 | N | TYR | 73 | 60.737 | 38.141 | 10.793 | 1.00 | 18.10 | A_13 |
| ATOM | 669 | CA | TYR | 73 | 61.407 | 37.827 | 12.046 | 1.00 | 14.01 | A_13 |
| ATOM | 670 | CB | TYR | 73 | 62.845 | 37.331 | 11.803 | 1.00 | 21.08 | A_13 |
| ATOM | 671 | CG | TYR | 73 | 62.915 | 35.965 | 11.138 | 1.00 | 22.48 | A_13 |
| ATOM | 672 | CD1 | TYR | 73 | 63.579 | 35.788 | 9.923 | 1.00 | 30.23 | A_13 |
| ATOM | 673 | CE1 | TYR | 73 | 63.615 | 34.538 | 9.291 | 1.00 | 24.04 | A_13 |
| ATOM | 674 | CD2 | TYR | 73 | 62.288 | 34.856 | 11.710 | 1.00 | 19.23 | A_13 |
| ATOM | 675 | CE2 | TYR | 73 | 62.320 | 33.606 | 11.083 | 1.00 | 29.35 | A_13 |
| ATOM | 676 | CZ | TYR | 73 | 62.984 | 33.460 | 9.875 | 1.00 | 12.50 | A_13 |
| ATOM | 677 | OH | TYR | 73 | 63.018 | 32.246 | 9.241 | 1.00 | 17.89 | A_13 |
| ATOM | 679 | C | TYR | 73 | 61.360 | 39.203 | 12.721 | 1.00 | 22.00 | A_13 |
| ATOM | 680 | O | TYR | 73 | 62.365 | 39.919 | 12.819 | 1.00 | 10.93 | A_13 |
| ATOM | 681 | N | PRO | 74 | 60.175 | 39.570 | 13.221 | 1.00 | 19.94 | A_13 |
| ATOM | 682 | CD | PRO | 74 | 58.969 | 38.723 | 13.278 | 1.00 | 15.69 | A_13 |
| ATOM | 683 | CA | PRO | 74 | 59.934 | 40.843 | 13.886 | 1.00 | 16.75 | A_13 |
| ATOM | 684 | CB | PRO | 74 | 58.417 | 40.836 | 14.067 | 1.00 | 17.27 | A_13 |
| ATOM | 685 | CG | PRO | 74 | 58.131 | 39.407 | 14.335 | 1.00 | 16.24 | A_13 |
| ATOM | 686 | C | PRO | 74 | 60.640 | 41.037 | 15.216 | 1.00 | 17.39 | A_13 |
| ATOM | 687 | O | PRO | 74 | 60.779 | 40.105 | 16.023 | 1.00 | 10.00 | A_13 |
| ATOM | 688 | N | PHE | 75 | 61.098 | 42.264 | 15.431 | 1.00 | 10.00 | A_13 |
| ATOM | 690 | CA | PHE | 75 | 61.743 | 42.618 | 16.675 | 1.00 | 16.45 | A_13 |
| ATOM | 691 | CB | PHE | 75 | 62.613 | 43.865 | 16.512 | 1.00 | 20.71 | A_13 |
| ATOM | 692 | CG | PHE | 75 | 63.931 | 43.590 | 15.841 | 1.00 | 23.32 | A_13 |
| ATOM | 693 | CD1 | PHE | 75 | 64.694 | 42.482 | 16.200 | 1.00 | 12.03 | A_13 |
| ATOM | 694 | CD2 | PHE | 75 | 64.405 | 44.420 | 14.842 | 1.00 | 22.30 | A_13 |
| ATOM | 695 | CE1 | PHE | 75 | 65.905 | 42.214 | 15.572 | 1.00 | 17.64 | A_13 |
| ATOM | 696 | CE2 | PHE | 75 | 65.622 | 44.148 | 14.208 | 1.00 | 15.43 | A_13 |
| ATOM | 697 | CZ | PHE | 75 | 66.367 | 43.044 | 14.576 | 1.00 | 10.00 | A_13 |
| ATOM | 698 | C | PHE | 75 | 60.632 | 42.784 | 17.707 | 1.00 | 25.73 | A_13 |
| ATOM | 699 | O | PHE | 75 | 59.443 | 42.778 | 17.370 | 1.00 | 18.57 | A_13 |
| ATOM | 700 | N | ASP | 76 | 61.009 | 43.002 | 18.952 | 1.00 | 20.50 | A_13 |
| ATOM | 702 | CA | ASP | 76 | 60.023 | 43.049 | 20.006 | 1.00 | 13.89 | A_13 |
| ATOM | 703 | CB | ASP | 76 | 60.241 | 41.805 | 20.873 | 1.00 | 20.69 | A_13 |
| ATOM | 704 | CG | ASP | 76 | 61.672 | 41.685 | 21.378 | 1.00 | 22.52 | A_13 |
| ATOM | 705 | OD1 | ASP | 76 | 61.947 | 40.771 | 22.174 | 1.00 | 20.06 | A_13 |
| ATOM | 706 | OD2 | ASP | 76 | 62.525 | 42.506 | 20.998 | 1.00 | 10.69 | A_13 |
| ATOM | 707 | C | ASP | 76 | 59.971 | 44.277 | 20.900 | 1.00 | 25.20 | A_13 |
| ATOM | 708 | O | ASP | 76 | 59.397 | 44.207 | 21.986 | 1.00 | 29.52 | A_13 |
| ATOM | 709 | N | GLY | 77 | 60.585 | 45.379 | 20.488 | 1.00 | 10.00 | A_13 |
| ATOM | 711 | CA | GLY | 77 | 60.575 | 46.553 | 21.334 | 1.00 | 10.00 | A_13 |
| ATOM | 712 | C | GLY | 77 | 61.769 | 46.514 | 22.266 | 1.00 | 10.00 | A_13 |
| ATOM | 713 | O | GLY | 77 | 62.735 | 45.797 | 21.987 | 1.00 | 18.49 | A_13 |
| ATOM | 714 | N | PRO | 78 | 61.785 | 47.344 | 23.322 | 1.00 | 16.07 | A_13 |
| ATOM | 715 | CD | PRO | 78 | 60.790 | 48.426 | 23.505 | 1.00 | 15.88 | A_13 |
| ATOM | 716 | CA | PRO | 78 | 62.855 | 47.439 | 24.330 | 1.00 | 16.23 | A_13 |
| ATOM | 717 | CB | PRO | 78 | 62.261 | 48.391 | 25.363 | 1.00 | 22.96 | A_13 |
| ATOM | 718 | CG | PRO | 78 | 61.470 | 49.349 | 24.501 | 1.00 | 22.37 | A_13 |
| ATOM | 719 | C | PRO | 78 | 63.150 | 46.090 | 24.969 | 1.00 | 25.32 | A_13 |
| ATOM | 720 | O | PRO | 78 | 62.227 | 45.356 | 25.272 | 1.00 | 20.04 | A_13 |
| ATOM | 721 | N | SER | 79 | 64.432 | 45.750 | 25.099 | 1.00 | 20.93 | A_13 |
| ATOM | 723 | CA | SER | 79 | 64.878 | 44.478 | 25.689 | 1.00 | 20.51 | A_13 |
| ATOM | 724 | CB | SER | 79 | 64.364 | 44.311 | 27.131 | 1.00 | 23.69 | A_13 |
| ATOM | 725 | OG | SER | 79 | 65.028 | 45.211 | 28.006 | 1.00 | 33.37 | A_13 |
| ATOM | 727 | C | SER | 79 | 64.557 | 43.248 | 24.863 | 1.00 | 20.39 | A_13 |
| ATOM | 728 | O | SER | 79 | 64.124 | 43.362 | 23.708 | 1.00 | 17.27 | A_13 |
| ATOM | 729 | N | GLY | 80 | 64.825 | 42.071 | 25.415 | 1.00 | 13.38 | A_13 |
| ATOM | 731 | CA | GLY | 80 | 64.564 | 40.850 | 24.678 | 1.00 | 10.11 | A_13 |
| ATOM | 732 | C | GLY | 80 | 65.471 | 40.808 | 23.458 | 1.00 | 13.15 | A_13 |
| ATOM | 733 | O | GLY | 80 | 66.614 | 41.251 | 23.538 | 1.00 | 31.80 | A_13 |
| ATOM | 734 | N | LEU | 81 | 64.939 | 40.393 | 22.310 | 1.00 | 29.05 | A_13 |
| ATOM | 736 | CA | LEU | 81 | 65.720 | 40.317 | 21.078 | 1.00 | 29.63 | A_13 |
| ATOM | 737 | CB | LEU | 81 | 64.789 | 40.033 | 19.905 | 1.00 | 19.67 | A_13 |
| ATOM | 738 | CG | LEU | 81 | 65.121 | 38.872 | 18.971 | 1.00 | 21.79 | A_13 |
| ATOM | 739 | CD1 | LEU | 81 | 64.215 | 38.980 | 17.773 | 1.00 | 23.87 | A_13 |
| ATOM | 740 | CD2 | LEU | 81 | 66.590 | 38.918 | 18.518 | 1.00 | 22.09 | A_13 |
| ATOM | 741 | C | LEU | 81 | 66.442 | 41.649 | 20.835 | 1.00 | 19.25 | A_13 |
| ATOM | 742 | O | LEU | 81 | 65.808 | 42.700 | 20.872 | 1.00 | 14.95 | A_13 |
| ATOM | 743 | N | LEU | 82 | 67.760 | 41.599 | 20.657 | 1.00 | 25.03 | A_13 |
| ATOM | 745 | CA | LEU | 82 | 68.573 | 42.795 | 20.421 | 1.00 | 27.35 | A_13 |
| ATOM | 746 | CB | LEU | 82 | 69.868 | 42.747 | 21.244 | 1.00 | 12.74 | A_13 |
| ATOM | 747 | CG | LEU | 82 | 69.802 | 42.748 | 22.773 | 1.00 | 16.50 | A_13 |
| ATOM | 748 | CD1 | LEU | 82 | 68.590 | 43.520 | 23.263 | 1.00 | 17.99 | A_13 |

45/75

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 749 | CD2 | LEU | 82 | 69.744 | 41.343 | 23.279 | 1.00 | 13.28 | A_13 |
| ATOM | 750 | C | LEU | 82 | 68.938 | 42.945 | 18.949 | 1.00 | 24.79 | A_13 |
| ATOM | 751 | O | LEU | 82 | 68.812 | 44.039 | 18.363 | 1.00 | 14.36 | A_13 |
| ATOM | 752 | N | ALA | 83 | 69.387 | 41.839 | 18.359 | 1.00 | 21.15 | A_13 |
| ATOM | 754 | CA | ALA | 83 | 69.790 | 41.819 | 16.961 | 1.00 | 15.64 | A_13 |
| ATOM | 755 | CB | ALA | 83 | 71.180 | 42.410 | 16.820 | 1.00 | 15.74 | A_13 |
| ATOM | 756 | C | ALA | 83 | 69.806 | 40.400 | 16.444 | 1.00 | 19.37 | A_13 |
| ATOM | 757 | O | ALA | 83 | 69.864 | 39.458 | 17.227 | 1.00 | 20.42 | A_13 |
| ATOM | 758 | N | HIS | 84 | 69.746 | 40.252 | 15.126 | 1.00 | 10.72 | A_13 |
| ATOM | 760 | CA | HIS | 84 | 69.808 | 38.939 | 14.502 | 1.00 | 20.51 | A_13 |
| ATOM | 761 | CB | HIS | 84 | 68.454 | 38.185 | 14.476 | 1.00 | 12.34 | A_13 |
| ATOM | 762 | CG | HIS | 84 | 67.361 | 38.849 | 13.679 | 1.00 | 24.79 | A_13 |
| ATOM | 763 | CD2 | HIS | 84 | 67.381 | 39.489 | 12.488 | 1.00 | 10.00 | A_13 |
| ATOM | 764 | ND1 | HIS | 84 | 66.052 | 38.869 | 14.104 | 1.00 | 13.50 | A_13 |
| ATOM | 766 | CE1 | HIS | 84 | 65.307 | 39.497 | 13.210 | 1.00 | 14.37 | A_13 |
| ATOM | 767 | NE2 | HIS | 84 | 66.087 | 39.886 | 12.220 | 1.00 | 15.00 | A_13 |
| ATOM | 768 | C | HIS | 84 | 70.418 | 39.088 | 13.130 | 1.00 | 22.78 | A_13 |
| ATOM | 769 | O | HIS | 84 | 70.338 | 40.162 | 12.532 | 1.00 | 10.00 | A_13 |
| ATOM | 770 | N | ALA | 85 | 71.086 | 38.027 | 12.685 | 1.00 | 13.43 | A_13 |
| ATOM | 772 | CA | ALA | 85 | 71.746 | 37.983 | 11.402 | 1.00 | 10.00 | A_13 |
| ATOM | 773 | CB | ALA | 85 | 73.234 | 38.132 | 11.596 | 1.00 | 10.05 | A_13 |
| ATOM | 774 | C | ALA | 85 | 71.426 | 36.661 | 10.721 | 1.00 | 17.89 | A_13 |
| ATOM | 775 | O | ALA | 85 | 70.900 | 35.746 | 11.346 | 1.00 | 19.43 | A_13 |
| ATOM | 776 | N | PHE | 86 | 71.697 | 36.585 | 9.425 | 1.00 | 13.49 | A_13 |
| ATOM | 778 | CA | PHE | 86 | 71.459 | 35.372 | 8.651 | 1.00 | 12.49 | A_13 |
| ATOM | 779 | CB | PHE | 86 | 70.739 | 35.728 | 7.344 | 1.00 | 10.00 | A_13 |
| ATOM | 780 | CG | PHE | 86 | 69.348 | 36.240 | 7.529 | 1.00 | 19.96 | A_13 |
| ATOM | 781 | CD1 | PHE | 86 | 68.252 | 35.434 | 7.212 | 1.00 | 21.89 | A_13 |
| ATOM | 782 | CD2 | PHE | 86 | 69.119 | 37.530 | 8.003 | 1.00 | 10.63 | A_13 |
| ATOM | 783 | CE1 | PHE | 86 | 66.946 | 35.900 | 7.364 | 1.00 | 16.59 | A_13 |
| ATOM | 784 | CE2 | PHE | 86 | 67.829 | 38.009 | 8.158 | 1.00 | 19.06 | A_13 |
| ATOM | 785 | CZ | PHE | 86 | 66.732 | 37.194 | 7.838 | 1.00 | 24.79 | A_13 |
| ATOM | 786 | C | PHE | 86 | 72.802 | 34.721 | 8.298 | 1.00 | 11.05 | A_13 |
| ATOM | 787 | O | PHE | 86 | 73.774 | 35.435 | 8.041 | 1.00 | 25.56 | A_13 |
| ATOM | 788 | N | PRO | 87 | 72.892 | 33.375 | 8.304 | 1.00 | 19.41 | A_13 |
| ATOM | 789 | CD | PRO | 87 | 71.876 | 32.383 | 8.717 | 1.00 | 17.25 | A_13 |
| ATOM | 790 | CA | PRO | 87 | 74.149 | 32.686 | 7.956 | 1.00 | 29.29 | A_13 |
| ATOM | 791 | CB | PRO | 87 | 73.800 | 31.198 | 8.135 | 1.00 | 18.88 | A_13 |
| ATOM | 792 | CG | PRO | 87 | 72.329 | 31.160 | 7.939 | 1.00 | 20.17 | A_13 |
| ATOM | 793 | C | PRO | 87 | 74.562 | 32.999 | 6.503 | 1.00 | 10.00 | A_13 |
| ATOM | 794 | O | PRO | 87 | 73.728 | 33.448 | 5.703 | 1.00 | 20.68 | A_13 |
| ATOM | 795 | N | PRO | 88 | 75.814 | 32.701 | 6.120 | 1.00 | 10.00 | A_13 |
| ATOM | 796 | CD | PRO | 88 | 76.796 | 31.854 | 6.831 | 1.00 | 19.58 | A_13 |
| ATOM | 797 | CA | PRO | 88 | 76.280 | 32.977 | 4.756 | 1.00 | 12.43 | A_13 |
| ATOM | 798 | CB | PRO | 88 | 77.600 | 32.201 | 4.676 | 1.00 | 18.69 | A_13 |
| ATOM | 799 | CG | PRO | 88 | 78.073 | 32.163 | 6.098 | 1.00 | 18.48 | A_13 |
| ATOM | 800 | C | PRO | 88 | 75.304 | 32.510 | 3.672 | 1.00 | 24.39 | A_13 |
| ATOM | 801 | O | PRO | 88 | 74.596 | 31.522 | 3.854 | 1.00 | 16.92 | A_13 |
| ATOM | 802 | N | GLY | 89 | 75.266 | 33.230 | 2.560 | 1.00 | 10.73 | A_13 |
| ATOM | 804 | CA | GLY | 89 | 74.386 | 32.868 | 1.471 | 1.00 | 10.00 | A_13 |
| ATOM | 805 | C | GLY | 89 | 73.960 | 34.127 | 0.772 | 1.00 | 10.94 | A_13 |
| ATOM | 806 | O | GLY | 89 | 74.143 | 35.218 | 1.307 | 1.00 | 19.86 | A_13 |
| ATOM | 807 | N | PRO | 90 | 73.390 | 34.019 | -0.432 | 1.00 | 26.31 | A_13 |
| ATOM | 808 | CD | PRO | 90 | 73.090 | 32.792 | -1.192 | 1.00 | 18.46 | A_13 |
| ATOM | 809 | CA | PRO | 90 | 72.960 | 35.212 | -1.163 | 1.00 | 25.07 | A_13 |
| ATOM | 810 | CB | PRO | 90 | 72.670 | 34.651 | -2.556 | 1.00 | 15.47 | A_13 |
| ATOM | 811 | CG | PRO | 90 | 72.108 | 33.289 | -2.236 | 1.00 | 24.63 | A_13 |
| ATOM | 812 | C | PRO | 90 | 71.726 | 35.879 | -0.543 | 1.00 | 20.41 | A_13 |
| ATOM | 813 | O | PRO | 90 | 71.176 | 35.390 | 0.442 | 1.00 | 17.00 | A_13 |
| ATOM | 814 | N | ASN | 91 | 71.303 | 37.000 | -1.125 | 1.00 | 18.43 | A_13 |
| ATOM | 816 | CA | ASN | 91 | 70.127 | 37.721 | -0.653 | 1.00 | 14.03 | A_13 |
| ATOM | 817 | CB | ASN | 91 | 68.863 | 36.932 | -0.999 | 1.00 | 15.26 | A_13 |
| ATOM | 818 | CG | ASN | 91 | 68.860 | 36.430 | -2.439 | 1.00 | 36.74 | A_13 |
| ATOM | 819 | OD1 | ASN | 91 | 68.497 | 35.282 | -2.701 | 1.00 | 29.56 | A_13 |
| ATOM | 820 | ND2 | ASN | 91 | 69.265 | 37.286 | -3.376 | 1.00 | 27.03 | A_13 |
| ATOM | 823 | C | ASN | 91 | 70.226 | 37.986 | 0.849 | 1.00 | 24.66 | A_13 |
| ATOM | 824 | O | ASN | 91 | 71.257 | 38.479 | 1.313 | 1.00 | 17.43 | A_13 |
| ATOM | 825 | N | TYR | 92 | 69.198 | 37.632 | 1.622 | 1.00 | 17.69 | A_13 |
| ATOM | 827 | CA | TYR | 92 | 69.233 | 37.876 | 3.061 | 1.00 | 10.17 | A_13 |
| ATOM | 828 | CB | TYR | 92 | 67.942 | 37.428 | 3.744 | 1.00 | 16.78 | A_13 |
| ATOM | 829 | CG | TYR | 92 | 66.786 | 38.364 | 3.523 | 1.00 | 26.17 | A_13 |
| ATOM | 830 | CD1 | TYR | 92 | 66.015 | 38.803 | 4.581 | 1.00 | 17.79 | A_13 |
| ATOM | 831 | CE1 | TYR | 92 | 64.947 | 39.678 | 4.380 | 1.00 | 29.60 | A_13 |
| ATOM | 832 | CD2 | TYR | 92 | 66.467 | 38.818 | 2.250 | 1.00 | 25.90 | A_13 |
| ATOM | 833 | CE2 | TYR | 92 | 65.406 | 39.691 | 2.040 | 1.00 | 30.60 | A_13 |
| ATOM | 834 | CZ | TYR | 92 | 64.647 | 40.117 | 3.107 | 1.00 | 12.31 | A_13 |
| ATOM | 835 | OH | TYR | 92 | 63.575 | 40.967 | 2.886 | 1.00 | 26.07 | A_13 |

46/75

| | | | | | | | | | | |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 837 | C | TYR | 92 | 70.427 | 37.245 | 3.763 | 1.00 | 11.94 | A_13 |
| ATOM | 838 | O | TYR | 92 | 70.752 | 37.617 | 4.882 | 1.00 | 17.58 | A_13 |
| ATOM | 839 | N | GLY | 93 | 71.095 | 36.311 | 3.097 | 1.00 | 24.67 | A_13 |
| ATOM | 841 | CA | GLY | 93 | 72.250 | 35.666 | 3.691 | 1.00 | 18.05 | A_13 |
| ATOM | 842 | C | GLY | 93 | 73.295 | 36.681 | 4.116 | 1.00 | 10.00 | A_13 |
| ATOM | 843 | O | GLY | 93 | 73.573 | 37.656 | 3.391 | 1.00 | 10.13 | A_13 |
| ATOM | 844 | N | GLY | 94 | 73.812 | 36.495 | 5.328 | 1.00 | 12.44 | A_13 |
| ATOM | 846 | CA | GLY | 94 | 74.827 | 37.372 | 5.872 | 1.00 | 10.00 | A_13 |
| ATOM | 847 | C | GLY | 94 | 74.358 | 38.694 | 6.456 | 1.00 | 17.29 | A_13 |
| ATOM | 848 | O | GLY | 94 | 75.052 | 39.271 | 7.284 | 1.00 | 14.53 | A_13 |
| ATOM | 849 | N | ASP | 95 | 73.221 | 39.206 | 5.993 | 1.00 | 10.00 | A_13 |
| ATOM | 851 | CA | ASP | 95 | 72.689 | 40.485 | 6.472 | 1.00 | 16.35 | A_13 |
| ATOM | 852 | CB | ASP | 95 | 71.332 | 40.777 | 5.814 | 1.00 | 10.00 | A_13 |
| ATOM | 853 | CG | ASP | 95 | 71.421 | 40.904 | 4.309 | 1.00 | 14.54 | A_13 |
| ATOM | 854 | OD1 | ASP | 95 | 70.406 | 41.256 | 3.673 | 1.00 | 11.86 | A_13 |
| ATOM | 855 | OD2 | ASP | 95 | 72.502 | 40.647 | 3.753 | 1.00 | 15.39 | A_13 |
| ATOM | 856 | C | ASP | 95 | 72.548 | 40.523 | 7.994 | 1.00 | 22.31 | A_13 |
| ATOM | 857 | O | ASP | 95 | 72.279 | 39.497 | 8.635 | 1.00 | 10.88 | A_13 |
| ATOM | 858 | N | ALA | 96 | 72.703 | 41.711 | 8.566 | 1.00 | 18.45 | A_13 |
| ATOM | 860 | CA | ALA | 96 | 72.609 | 41.877 | 10.011 | 1.00 | 15.08 | A_13 |
| ATOM | 861 | CB | ALA | 96 | 73.982 | 42.244 | 10.587 | 1.00 | 19.20 | A_13 |
| ATOM | 862 | C | ALA | 96 | 71.587 | 42.961 | 10.345 | 1.00 | 14.91 | A_13 |
| ATOM | 863 | O | ALA | 96 | 71.702 | 44.092 | 9.876 | 1.00 | 10.00 | A_13 |
| ATOM | 864 | N | HIS | 97 | 70.635 | 42.646 | 11.215 | 1.00 | 14.01 | A_13 |
| ATOM | 866 | CA | HIS | 97 | 69.599 | 43.620 | 11.581 | 1.00 | 11.35 | A_13 |
| ATOM | 867 | CB | HIS | 97 | 68.207 | 43.083 | 11.203 | 1.00 | 20.32 | A_13 |
| ATOM | 868 | CG | HIS | 97 | 68.027 | 42.786 | 9.742 | 1.00 | 15.00 | A_13 |
| ATOM | 869 | CD2 | HIS | 97 | 68.734 | 43.186 | 8.654 | 1.00 | 10.00 | A_13 |
| ATOM | 870 | ND1 | HIS | 97 | 67.014 | 41.978 | 9.257 | 1.00 | 14.03 | A_13 |
| ATOM | 871 | CE1 | HIS | 97 | 67.108 | 41.895 | 7.936 | 1.00 | 10.00 | A_13 |
| ATOM | 872 | NE2 | HIS | 97 | 68.142 | 42.618 | 7.552 | 1.00 | 17.10 | A_13 |
| ATOM | 874 | C | HIS | 97 | 69.650 | 43.952 | 13.078 | 1.00 | 13.37 | A_13 |
| ATOM | 875 | O | HIS | 97 | 69.736 | 43.055 | 13.908 | 1.00 | 13.48 | A_13 |
| ATOM | 876 | N | PHE | 98 | 69.596 | 45.237 | 13.423 | 1.00 | 21.01 | A_13 |
| ATOM | 878 | CA | PHE | 98 | 69.634 | 45.668 | 14.823 | 1.00 | 11.27 | A_13 |
| ATOM | 879 | CB | PHE | 98 | 70.817 | 46.615 | 15.055 | 1.00 | 10.00 | A_13 |
| ATOM | 880 | CG | PHE | 98 | 72.138 | 46.011 | 14.703 | 1.00 | 20.49 | A_13 |
| ATOM | 881 | CD1 | PHE | 98 | 72.984 | 45.524 | 15.707 | 1.00 | 17.49 | A_13 |
| ATOM | 882 | CD2 | PHE | 98 | 72.506 | 45.853 | 13.365 | 1.00 | 13.51 | A_13 |
| ATOM | 883 | CE1 | PHE | 98 | 74.171 | 44.888 | 15.382 | 1.00 | 20.00 | A_13 |
| ATOM | 884 | CE2 | PHE | 98 | 73.693 | 45.215 | 13.024 | 1.00 | 10.00 | A_13 |
| ATOM | 885 | CZ | PHE | 98 | 74.527 | 44.728 | 14.029 | 1.00 | 10.00 | A_13 |
| ATOM | 886 | C | PHE | 98 | 68.336 | 46.336 | 15.245 | 1.00 | 25.38 | A_13 |
| ATOM | 887 | O | PHE | 98 | 67.815 | 47.218 | 14.552 | 1.00 | 10.00 | A_13 |
| ATOM | 888 | N | ASP | 99 | 67.817 | 45.924 | 16.394 | 1.00 | 21.68 | A_13 |
| ATOM | 890 | CA | ASP | 99 | 66.567 | 46.476 | 16.886 | 1.00 | 10.00 | A_13 |
| ATOM | 891 | CB | ASP | 99 | 66.039 | 45.604 | 18.010 | 1.00 | 10.00 | A_13 |
| ATOM | 892 | CG | ASP | 99 | 64.648 | 45.998 | 18.473 | 1.00 | 14.00 | A_13 |
| ATOM | 893 | OD1 | ASP | 99 | 64.104 | 45.272 | 19.329 | 1.00 | 15.19 | A_13 |
| ATOM | 894 | OD2 | ASP | 99 | 64.089 | 47.011 | 18.001 | 1.00 | 17.01 | A_13 |
| ATOM | 895 | C | ASP | 99 | 66.817 | 47.871 | 17.391 | 1.00 | 13.06 | A_13 |
| ATOM | 896 | O | ASP | 99 | 67.528 | 48.056 | 18.374 | 1.00 | 10.00 | A_13 |
| ATOM | 897 | N | ASP | 100 | 66.203 | 48.856 | 16.746 | 1.00 | 15.56 | A_13 |
| ATOM | 899 | CA | ASP | 100 | 66.397 | 50.232 | 17.177 | 1.00 | 18.23 | A_13 |
| ATOM | 900 | CB | ASP | 100 | 66.121 | 51.228 | 16.041 | 1.00 | 15.05 | A_13 |
| ATOM | 901 | CG | ASP | 100 | 67.275 | 52.180 | 15.838 | 1.00 | 11.67 | A_13 |
| ATOM | 902 | OD1 | ASP | 100 | 67.602 | 52.516 | 14.683 | 1.00 | 21.07 | A_13 |
| ATOM | 903 | OD2 | ASP | 100 | 67.879 | 52.569 | 16.860 | 1.00 | 14.72 | A_13 |
| ATOM | 904 | C | ASP | 100 | 65.610 | 50.572 | 18.445 | 1.00 | 10.00 | A_13 |
| ATOM | 905 | O | ASP | 100 | 65.767 | 51.635 | 19.009 | 1.00 | 17.18 | A_13 |
| ATOM | 906 | N | ASP | 101 | 64.755 | 49.669 | 18.895 | 1.00 | 14.57 | A_13 |
| ATOM | 908 | CA | ASP | 101 | 64.031 | 49.924 | 20.123 | 1.00 | 17.59 | A_13 |
| ATOM | 909 | CB | ASP | 101 | 62.769 | 49.051 | 20.236 | 1.00 | 12.50 | A_13 |
| ATOM | 910 | CG | ASP | 101 | 61.532 | 49.721 | 19.606 | 1.00 | 17.12 | A_13 |
| ATOM | 911 | OD1 | ASP | 101 | 60.599 | 49.023 | 19.179 | 1.00 | 10.39 | A_13 |
| ATOM | 912 | OD2 | ASP | 101 | 61.480 | 50.962 | 19.536 | 1.00 | 18.09 | A_13 |
| ATOM | 913 | C | ASP | 101 | 64.994 | 49.766 | 21.306 | 1.00 | 19.33 | A_13 |
| ATOM | 914 | O | ASP | 101 | 64.610 | 49.972 | 22.456 | 1.00 | 10.00 | A_13 |
| ATOM | 915 | N | GLU | 102 | 66.213 | 49.301 | 21.019 | 1.00 | 16.15 | A_13 |
| ATOM | 917 | CA | GLU | 102 | 67.267 | 49.194 | 22.044 | 1.00 | 13.43 | A_13 |
| ATOM | 918 | CB | GLU | 102 | 68.264 | 48.085 | 21.720 | 1.00 | 18.25 | A_13 |
| ATOM | 919 | CG | GLU | 102 | 67.697 | 46.704 | 21.636 | 1.00 | 10.00 | A_13 |
| ATOM | 920 | CD | GLU | 102 | 66.650 | 46.467 | 22.672 | 1.00 | 11.18 | A_13 |
| ATOM | 921 | OE1 | GLU | 102 | 66.872 | 46.746 | 23.870 | 1.00 | 16.09 | A_13 |
| ATOM | 922 | OE2 | GLU | 102 | 65.572 | 46.033 | 22.271 | 1.00 | 26.76 | A_13 |
| ATOM | 923 | C | GLU | 102 | 68.070 | 50.495 | 22.007 | 1.00 | 11.07 | A_13 |
| ATOM | 924 | O | GLU | 102 | 68.103 | 51.161 | 20.971 | 1.00 | 13.97 | A_13 |

47/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 925 | N | THR | 103 | 68.774 | 50.823 | 23.091 | 1.00 | 22.82 | A_13 |
| ATOM | 927 | CA | THR | 103 | 69.606 | 52.034 | 23.102 | 1.00 | 13.45 | A_13 |
| ATOM | 928 | CB | THR | 103 | 69.571 | 52.793 | 24.459 | 1.00 | 20.78 | A_13 |
| ATOM | 929 | OG1 | THR | 103 | 68.236 | 53.228 | 24.745 | 1.00 | 10.69 | A_13 |
| ATOM | 931 | CG2 | THR | 103 | 70.445 | 54.046 | 24.378 | 1.00 | 19.45 | A_13 |
| ATOM | 932 | C | THR | 103 | 71.030 | 51.571 | 22.822 | 1.00 | 12.42 | A_13 |
| ATOM | 933 | O | THR | 103 | 71.639 | 50.896 | 23.642 | 1.00 | 19.81 | A_13 |
| ATOM | 934 | N | TRP | 104 | 71.525 | 51.854 | 21.626 | 1.00 | 10.00 | A_13 |
| ATOM | 936 | CA | TRP | 104 | 72.873 | 51.448 | 21.248 | 1.00 | 13.61 | A_13 |
| ATOM | 937 | CB | TRP | 104 | 72.943 | 51.221 | 19.739 | 1.00 | 29.21 | A_13 |
| ATOM | 938 | CG | TRP | 104 | 71.970 | 50.174 | 19.313 | 1.00 | 21.39 | A_13 |
| ATOM | 939 | CD2 | TRP | 104 | 72.101 | 48.760 | 19.501 | 1.00 | 25.13 | A_13 |
| ATOM | 940 | CE2 | TRP | 104 | 70.937 | 48.156 | 18.964 | 1.00 | 28.84 | A_13 |
| ATOM | 941 | CE3 | TRP | 104 | 73.088 | 47.941 | 20.070 | 1.00 | 13.36 | A_13 |
| ATOM | 942 | CD1 | TRP | 104 | 70.765 | 50.372 | 18.694 | 1.00 | 21.59 | A_13 |
| ATOM | 943 | NE1 | TRP | 104 | 70.139 | 49.163 | 18.484 | 1.00 | 19.91 | A_13 |
| ATOM | 945 | CZ2 | TRP | 104 | 70.738 | 46.768 | 18.977 | 1.00 | 10.00 | A_13 |
| ATOM | 946 | CZ3 | TRP | 104 | 72.888 | 46.568 | 20.084 | 1.00 | 14.54 | A_13 |
| ATOM | 947 | CH2 | TRP | 104 | 71.720 | 45.995 | 19.539 | 1.00 | 11.93 | A_13 |
| ATOM | 948 | C | TRP | 104 | 73.912 | 52.453 | 21.725 | 1.00 | 16.59 | A_13 |
| ATOM | 949 | O | TRP | 104 | 73.707 | 53.671 | 21.642 | 1.00 | 12.90 | A_13 |
| ATOM | 950 | N | THR | 105 | 75.013 | 51.949 | 22.268 | 1.00 | 20.85 | A_13 |
| ATOM | 952 | CA | THR | 105 | 76.040 | 52.831 | 22.794 | 1.00 | 12.38 | A_13 |
| ATOM | 953 | CB | THR | 105 | 75.974 | 52.890 | 24.322 | 1.00 | 14.39 | A_13 |
| ATOM | 954 | OG1 | THR | 105 | 76.345 | 51.609 | 24.849 | 1.00 | 16.42 | A_13 |
| ATOM | 956 | CG2 | THR | 105 | 74.575 | 53.273 | 24.797 | 1.00 | 12.17 | A_13 |
| ATOM | 957 | C | THR | 105 | 77.437 | 52.378 | 22.457 | 1.00 | 10.00 | A_13 |
| ATOM | 958 | O | THR | 105 | 77.644 | 51.261 | 22.012 | 1.00 | 18.98 | A_13 |
| ATOM | 959 | N | SER | 106 | 78.385 | 53.277 | 22.704 | 1.00 | 26.01 | A_13 |
| ATOM | 961 | CA | SER | 106 | 79.809 | 53.043 | 22.502 | 1.00 | 17.80 | A_13 |
| ATOM | 962 | CB | SER | 106 | 80.466 | 54.284 | 21.888 | 1.00 | 20.63 | A_13 |
| ATOM | 963 | OG | SER | 106 | 79.744 | 54.756 | 20.763 | 1.00 | 38.89 | A_13 |
| ATOM | 965 | C | SER | 106 | 80.435 | 52.779 | 23.880 | 1.00 | 34.75 | A_13 |
| ATOM | 966 | O | SER | 106 | 81.652 | 52.884 | 24.042 | 1.00 | 33.01 | A_13 |
| ATOM | 967 | N | SER | 107 | 79.590 | 52.494 | 24.875 | 1.00 | 25.87 | A_13 |
| ATOM | 969 | CA | SER | 107 | 80.032 | 52.221 | 26.240 | 1.00 | 19.68 | A_13 |
| ATOM | 970 | CB | SER | 107 | 80.082 | 53.510 | 27.061 | 1.00 | 23.47 | A_13 |
| ATOM | 971 | OG | SER | 107 | 78.819 | 54.158 | 27.096 | 1.00 | 33.70 | A_13 |
| ATOM | 973 | C | SER | 107 | 79.100 | 51.200 | 26.892 | 1.00 | 13.60 | A_13 |
| ATOM | 974 | O | SER | 107 | 78.460 | 50.418 | 26.193 | 1.00 | 16.40 | A_13 |
| ATOM | 975 | N | SER | 108 | 79.028 | 51.205 | 28.221 | 1.00 | 17.31 | A_13 |
| ATOM | 977 | CA | SER | 108 | 78.188 | 50.259 | 28.949 | 1.00 | 20.12 | A_13 |
| ATOM | 978 | CB | SER | 108 | 78.745 | 50.009 | 30.364 | 1.00 | 22.63 | A_13 |
| ATOM | 979 | OG | SER | 108 | 78.444 | 51.061 | 31.271 | 1.00 | 27.69 | A_13 |
| ATOM | 981 | C | SER | 108 | 76.702 | 50.606 | 29.076 | 1.00 | 19.98 | A_13 |
| ATOM | 982 | O | SER | 108 | 75.921 | 49.785 | 29.562 | 1.00 | 35.96 | A_13 |
| ATOM | 983 | N | LYS | 109 | 76.311 | 51.820 | 28.713 | 1.00 | 16.24 | A_13 |
| ATOM | 985 | CA | LYS | 109 | 74.907 | 52.186 | 28.847 | 1.00 | 11.10 | A_13 |
| ATOM | 986 | CB | LYS | 109 | 74.740 | 53.688 | 28.690 | 1.00 | 12.41 | A_13 |
| ATOM | 987 | CG | LYS | 109 | 73.555 | 54.239 | 29.462 | 1.00 | 32.67 | A_13 |
| ATOM | 988 | CD | LYS | 109 | 73.353 | 55.732 | 29.258 | 1.00 | 25.94 | A_13 |
| ATOM | 989 | CE | LYS | 109 | 74.535 | 56.599 | 29.749 | 1.00 | 25.11 | A_13 |
| ATOM | 990 | NZ | LYS | 109 | 74.225 | 58.070 | 29.636 | 1.00 | 22.70 | A_13 |
| ATOM | 994 | C | LYS | 109 | 74.138 | 51.424 | 27.773 | 1.00 | 21.67 | A_13 |
| ATOM | 995 | O | LYS | 109 | 74.667 | 51.210 | 26.694 | 1.00 | 32.76 | A_13 |
| ATOM | 996 | N | GLY | 110 | 72.932 | 50.955 | 28.081 | 1.00 | 29.60 | A_13 |
| ATOM | 998 | CA | GLY | 110 | 72.156 | 50.206 | 27.096 | 1.00 | 10.31 | A_13 |
| ATOM | 999 | C | GLY | 110 | 72.965 | 49.043 | 26.542 | 1.00 | 20.08 | A_13 |
| ATOM | 1000 | O | GLY | 110 | 73.672 | 48.362 | 27.285 | 1.00 | 11.17 | A_13 |
| ATOM | 1001 | N | TYR | 111 | 72.924 | 48.859 | 25.227 | 1.00 | 12.05 | A_13 |
| ATOM | 1003 | CA | TYR | 111 | 73.665 | 47.791 | 24.583 | 1.00 | 13.45 | A_13 |
| ATOM | 1004 | CB | TYR | 111 | 72.713 | 46.871 | 23.806 | 1.00 | 21.16 | A_13 |
| ATOM | 1005 | CG | TYR | 111 | 71.776 | 46.101 | 24.716 | 1.00 | 12.28 | A_13 |
| ATOM | 1006 | CD1 | TYR | 111 | 70.455 | 46.510 | 24.906 | 1.00 | 14.85 | A_13 |
| ATOM | 1007 | CE1 | TYR | 111 | 69.618 | 45.837 | 25.795 | 1.00 | 19.08 | A_13 |
| ATOM | 1008 | CD2 | TYR | 111 | 72.232 | 44.995 | 25.435 | 1.00 | 21.86 | A_13 |
| ATOM | 1009 | CE2 | TYR | 111 | 71.405 | 44.314 | 26.324 | 1.00 | 10.00 | A_13 |
| ATOM | 1010 | CZ | TYR | 111 | 70.101 | 44.740 | 26.505 | 1.00 | 18.51 | A_13 |
| ATOM | 1011 | OH | TYR | 111 | 69.282 | 44.077 | 27.398 | 1.00 | 14.32 | A_13 |
| ATOM | 1013 | C | TYR | 111 | 74.779 | 48.335 | 23.695 | 1.00 | 16.73 | A_13 |
| ATOM | 1014 | O | TYR | 111 | 74.540 | 49.105 | 22.764 | 1.00 | 11.98 | A_13 |
| ATOM | 1015 | N | ASN | 112 | 76.008 | 47.930 | 23.999 | 1.00 | 11.80 | A_13 |
| ATOM | 1017 | CA | ASN | 112 | 77.184 | 48.357 | 23.240 | 1.00 | 16.37 | A_13 |
| ATOM | 1018 | CB | ASN | 112 | 78.453 | 47.867 | 23.927 | 1.00 | 27.52 | A_13 |
| ATOM | 1019 | CG | ASN | 112 | 79.701 | 48.460 | 23.324 | 1.00 | 20.16 | A_13 |
| ATOM | 1020 | OD1 | ASN | 112 | 80.327 | 47.861 | 22.447 | 1.00 | 20.99 | A_13 |
| ATOM | 1021 | ND2 | ASN | 112 | 80.082 | 49.640 | 23.801 | 1.00 | 15.12 | A_13 |

48/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1024 | C | ASN | 112 | 77.137 | 47.809 | 21.813 | 1.00 | 18.08 | A_13 |
| ATOM | 1025 | O | ASN | 112 | 77.288 | 46.606 | 21.592 | 1.00 | 12.69 | A_13 |
| ATOM | 1026 | N | LEU | 113 | 76.972 | 48.700 | 20.844 | 1.00 | 11.15 | A_13 |
| ATOM | 1028 | CA | LEU | 113 | 76.878 | 48.296 | 19.461 | 1.00 | 10.00 | A_13 |
| ATOM | 1029 | CB | LEU | 113 | 76.718 | 49.526 | 18.568 | 1.00 | 10.24 | A_13 |
| ATOM | 1030 | CG | LEU | 113 | 76.325 | 49.262 | 17.106 | 1.00 | 15.67 | A_13 |
| ATOM | 1031 | CD1 | LEU | 113 | 75.155 | 48.296 | 17.050 | 1.00 | 26.54 | A_13 |
| ATOM | 1032 | CD2 | LEU | 113 | 75.967 | 50.555 | 16.415 | 1.00 | 15.60 | A_13 |
| ATOM | 1033 | C | LEU | 113 | 78.037 | 47.403 | 18.986 | 1.00 | 25.17 | A_13 |
| ATOM | 1034 | O | LEU | 113 | 77.799 | 46.380 | 18.336 | 1.00 | 17.24 | A_13 |
| ATOM | 1035 | N | PHE | 114 | 79.274 | 47.759 | 19.327 | 1.00 | 28.89 | A_13 |
| ATOM | 1037 | CA | PHE | 114 | 80.442 | 46.974 | 18.910 | 1.00 | 19.15 | A_13 |
| ATOM | 1038 | CB | PHE | 114 | 81.753 | 47.579 | 19.434 | 1.00 | 14.60 | A_13 |
| ATOM | 1039 | CG | PHE | 114 | 82.923 | 46.627 | 19.374 | 1.00 | 18.53 | A_13 |
| ATOM | 1040 | CD1 | PHE | 114 | 83.419 | 46.175 | 18.144 | 1.00 | 26.13 | A_13 |
| ATOM | 1041 | CD2 | PHE | 114 | 83.514 | 46.162 | 20.547 | 1.00 | 17.22 | A_13 |
| ATOM | 1042 | CE1 | PHE | 114 | 84.475 | 45.271 | 18.086 | 1.00 | 10.43 | A_13 |
| ATOM | 1043 | CE2 | PHE | 114 | 84.571 | 45.259 | 20.502 | 1.00 | 16.51 | A_13 |
| ATOM | 1044 | CZ | PHE | 114 | 85.052 | 44.815 | 19.260 | 1.00 | 15.54 | A_13 |
| ATOM | 1045 | C | PHE | 114 | 80.359 | 45.508 | 19.306 | 1.00 | 10.00 | A_13 |
| ATOM | 1046 | O | PHE | 114 | 80.437 | 44.625 | 18.445 | 1.00 | 33.07 | A_13 |
| ATOM | 1047 | N | LEU | 115 | 80.206 | 45.249 | 20.600 | 1.00 | 12.18 | A_13 |
| ATOM | 1049 | CA | LEU | 115 | 80.113 | 43.877 | 21.103 | 1.00 | 10.59 | A_13 |
| ATOM | 1050 | CB | LEU | 115 | 79.874 | 43.895 | 22.616 | 1.00 | 14.14 | A_13 |
| ATOM | 1051 | CG | LEU | 115 | 81.082 | 43.937 | 23.578 | 1.00 | 34.39 | A_13 |
| ATOM | 1052 | CD1 | LEU | 115 | 82.337 | 44.354 | 22.863 | 1.00 | 14.93 | A_13 |
| ATOM | 1053 | CD2 | LEU | 115 | 80.815 | 44.836 | 24.793 | 1.00 | 13.42 | A_13 |
| ATOM | 1054 | C | LEU | 115 | 79.019 | 43.080 | 20.379 | 1.00 | 12.06 | A_13 |
| ATOM | 1055 | O | LEU | 115 | 79.298 | 42.109 | 19.675 | 1.00 | 13.35 | A_13 |
| ATOM | 1056 | N | VAL | 116 | 77.786 | 43.558 | 20.459 | 1.00 | 13.11 | A_13 |
| ATOM | 1058 | CA | VAL | 116 | 76.678 | 42.875 | 19.814 | 1.00 | 12.97 | A_13 |
| ATOM | 1059 | CB | VAL | 116 | 75.343 | 43.569 | 20.129 | 1.00 | 28.07 | A_13 |
| ATOM | 1060 | CG1 | VAL | 116 | 74.200 | 42.926 | 19.340 | 1.00 | 17.32 | A_13 |
| ATOM | 1061 | CG2 | VAL | 116 | 75.074 | 43.491 | 21.617 | 1.00 | 22.14 | A_13 |
| ATOM | 1062 | C | VAL | 116 | 76.862 | 42.724 | 18.313 | 1.00 | 10.00 | A_13 |
| ATOM | 1063 | O | VAL | 116 | 76.473 | 41.716 | 17.755 | 1.00 | 14.68 | A_13 |
| ATOM | 1064 | N | ALA | 117 | 77.481 | 43.706 | 17.667 | 1.00 | 10.80 | A_13 |
| ATOM | 1066 | CA | ALA | 117 | 77.726 | 43.662 | 16.224 | 1.00 | 18.28 | A_13 |
| ATOM | 1067 | CB | ALA | 117 | 78.223 | 45.014 | 15.727 | 1.00 | 14.94 | A_13 |
| ATOM | 1068 | C | ALA | 117 | 78.735 | 42.579 | 15.863 | 1.00 | 25.24 | A_13 |
| ATOM | 1069 | O | ALA | 117 | 78.562 | 41.872 | 14.861 | 1.00 | 18.50 | A_13 |
| ATOM | 1070 | N | ALA | 118 | 79.795 | 42.458 | 16.665 | 1.00 | 24.40 | A_13 |
| ATOM | 1072 | CA | ALA | 118 | 80.829 | 41.451 | 16.422 | 1.00 | 11.80 | A_13 |
| ATOM | 1073 | CB | ALA | 118 | 81.945 | 41.590 | 17.447 | 1.00 | 19.28 | A_13 |
| ATOM | 1074 | C | ALA | 118 | 80.178 | 40.056 | 16.496 | 1.00 | 10.00 | A_13 |
| ATOM | 1075 | O | ALA | 118 | 80.426 | 39.183 | 15.660 | 1.00 | 10.00 | A_13 |
| ATOM | 1076 | N | HIS | 119 | 79.309 | 39.875 | 17.487 | 1.00 | 19.01 | A_13 |
| ATOM | 1078 | CA | HIS | 119 | 78.587 | 38.624 | 17.674 | 1.00 | 14.36 | A_13 |
| ATOM | 1079 | CB | HIS | 119 | 77.725 | 38.751 | 18.924 | 1.00 | 10.00 | A_13 |
| ATOM | 1080 | CG | HIS | 119 | 76.796 | 37.602 | 19.166 | 1.00 | 10.00 | A_13 |
| ATOM | 1081 | CD2 | HIS | 119 | 75.691 | 37.187 | 18.498 | 1.00 | 14.94 | A_13 |
| ATOM | 1082 | ND1 | HIS | 119 | 76.905 | 36.783 | 20.263 | 1.00 | 20.37 | A_13 |
| ATOM | 1084 | CE1 | HIS | 119 | 75.917 | 35.909 | 20.270 | 1.00 | 17.53 | A_13 |
| ATOM | 1085 | NE2 | HIS | 119 | 75.161 | 36.134 | 19.208 | 1.00 | 17.55 | A_13 |
| ATOM | 1086 | C | HIS | 119 | 77.741 | 38.339 | 16.419 | 1.00 | 10.00 | A_13 |
| ATOM | 1087 | O | HIS | 119 | 77.779 | 37.245 | 15.856 | 1.00 | 10.64 | A_13 |
| ATOM | 1088 | N | GLU | 120 | 77.004 | 39.343 | 15.968 | 1.00 | 22.95 | A_13 |
| ATOM | 1090 | CA | GLU | 120 | 76.174 | 39.224 | 14.775 | 1.00 | 23.96 | A_13 |
| ATOM | 1091 | CB | GLU | 120 | 75.429 | 40.545 | 14.502 | 1.00 | 17.19 | A_13 |
| ATOM | 1092 | CG | GLU | 120 | 74.373 | 40.889 | 15.555 | 1.00 | 16.14 | A_13 |
| ATOM | 1093 | CD | GLU | 120 | 73.492 | 39.691 | 15.929 | 1.00 | 10.00 | A_13 |
| ATOM | 1094 | OE1 | GLU | 120 | 73.478 | 39.354 | 17.122 | 1.00 | 17.94 | A_13 |
| ATOM | 1095 | OE2 | GLU | 120 | 72.844 | 39.078 | 15.047 | 1.00 | 17.03 | A_13 |
| ATOM | 1096 | C | GLU | 120 | 76.992 | 38.832 | 13.549 | 1.00 | 11.45 | A_13 |
| ATOM | 1097 | O | GLU | 120 | 76.594 | 37.946 | 12.772 | 1.00 | 13.34 | A_13 |
| ATOM | 1098 | N | PHE | 121 | 78.127 | 39.498 | 13.353 | 1.00 | 10.00 | A_13 |
| ATOM | 1100 | CA | PHE | 121 | 78.959 | 39.187 | 12.216 | 1.00 | 14.70 | A_13 |
| ATOM | 1101 | CB | PHE | 121 | 80.040 | 40.245 | 12.039 | 1.00 | 10.00 | A_13 |
| ATOM | 1102 | CG | PHE | 121 | 79.481 | 41.623 | 11.792 | 1.00 | 21.57 | A_13 |
| ATOM | 1103 | CD1 | PHE | 121 | 80.235 | 42.764 | 12.069 | 1.00 | 16.73 | A_13 |
| ATOM | 1104 | CD2 | PHE | 121 | 78.164 | 41.788 | 11.331 | 1.00 | 13.91 | A_13 |
| ATOM | 1105 | CE1 | PHE | 121 | 79.682 | 44.054 | 11.891 | 1.00 | 11.69 | A_13 |
| ATOM | 1106 | CE2 | PHE | 121 | 77.615 | 43.066 | 11.152 | 1.00 | 18.93 | A_13 |
| ATOM | 1107 | CZ | PHE | 121 | 78.373 | 44.192 | 11.436 | 1.00 | 10.00 | A_13 |
| ATOM | 1108 | C | PHE | 121 | 79.505 | 37.756 | 12.283 | 1.00 | 17.14 | A_13 |
| ATOM | 1109 | O | PHE | 121 | 79.642 | 37.104 | 11.256 | 1.00 | 13.04 | A_13 |
| ATOM | 1110 | N | GLY | 122 | 79.738 | 37.245 | 13.490 | 1.00 | 16.60 | A_13 |

49/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1112 | CA | GLY | 122 | 80.202 | 35.872 | 13.627 | 1.00 | 19.45 | A_13 |
| ATOM | 1113 | C | GLY | 122 | 79.162 | 34.982 | 12.966 | 1.00 | 18.55 | A_13 |
| ATOM | 1114 | O | GLY | 122 | 79.500 | 33.988 | 12.306 | 1.00 | 10.03 | A_13 |
| ATOM | 1115 | N | HIS | 123 | 77.892 | 35.361 | 13.140 | 1.00 | 18.22 | A_13 |
| ATOM | 1117 | CA | HIS | 123 | 76.753 | 34.665 | 12.525 | 1.00 | 16.31 | A_13 |
| ATOM | 1118 | CB | HIS | 123 | 75.424 | 35.224 | 13.031 | 1.00 | 11.35 | A_13 |
| ATOM | 1119 | CG | HIS | 123 | 75.049 | 34.768 | 14.403 | 1.00 | 10.33 | A_13 |
| ATOM | 1120 | CD2 | HIS | 123 | 74.552 | 35.454 | 15.457 | 1.00 | 16.64 | A_13 |
| ATOM | 1121 | ND1 | HIS | 123 | 75.097 | 33.450 | 14.782 | 1.00 | 18.04 | A_13 |
| ATOM | 1123 | CE1 | HIS | 123 | 74.638 | 33.332 | 16.017 | 1.00 | 16.66 | A_13 |
| ATOM | 1124 | NE2 | HIS | 123 | 74.301 | 34.533 | 16.450 | 1.00 | 25.32 | A_13 |
| ATOM | 1125 | C | HIS | 123 | 76.771 | 34.853 | 10.997 | 1.00 | 13.66 | A_13 |
| ATOM | 1126 | O | HIS | 123 | 76.565 | 33.901 | 10.246 | 1.00 | 10.82 | A_13 |
| ATOM | 1127 | N | SER | 124 | 77.006 | 36.082 | 10.539 | 1.00 | 13.57 | A_13 |
| ATOM | 1129 | CA | SER | 124 | 77.030 | 36.368 | 9.099 | 1.00 | 12.03 | A_13 |
| ATOM | 1130 | CB | SER | 124 | 77.311 | 37.863 | 8.832 | 1.00 | 10.35 | A_13 |
| ATOM | 1131 | OG | SER | 124 | 76.399 | 38.706 | 9.510 | 1.00 | 14.26 | A_13 |
| ATOM | 1133 | C | SER | 124 | 78.117 | 35.548 | 8.422 | 1.00 | 21.45 | A_13 |
| ATOM | 1134 | O | SER | 124 | 78.079 | 35.333 | 7.210 | 1.00 | 10.00 | A_13 |
| ATOM | 1135 | N | LEU | 125 | 79.091 | 35.108 | 9.216 | 1.00 | 10.00 | A_13 |
| ATOM | 1137 | CA | LEU | 125 | 80.222 | 34.340 | 8.707 | 1.00 | 19.28 | A_13 |
| ATOM | 1138 | CB | LEU | 125 | 81.521 | 34.754 | 9.422 | 1.00 | 22.39 | A_13 |
| ATOM | 1139 | CG | LEU | 125 | 81.849 | 36.258 | 9.340 | 1.00 | 10.00 | A_13 |
| ATOM | 1140 | CD1 | LEU | 125 | 83.063 | 36.622 | 10.190 | 1.00 | 10.00 | A_13 |
| ATOM | 1141 | CD2 | LEU | 125 | 82.029 | 36.651 | 7.873 | 1.00 | 10.00 | A_13 |
| ATOM | 1142 | C | LEU | 125 | 79.986 | 32.851 | 8.843 | 1.00 | 10.00 | A_13 |
| ATOM | 1143 | O | LEU | 125 | 80.759 | 32.056 | 8.329 | 1.00 | 23.27 | A_13 |
| ATOM | 1144 | N | GLY | 126 | 78.932 | 32.477 | 9.563 | 1.00 | 22.87 | A_13 |
| ATOM | 1146 | CA | GLY | 126 | 78.604 | 31.070 | 9.720 | 1.00 | 17.27 | A_13 |
| ATOM | 1147 | C | GLY | 126 | 78.781 | 30.464 | 11.094 | 1.00 | 11.71 | A_13 |
| ATOM | 1148 | O | GLY | 126 | 78.784 | 29.244 | 11.236 | 1.00 | 24.16 | A_13 |
| ATOM | 1149 | N | LEU | 127 | 78.972 | 31.297 | 12.105 | 1.00 | 18.95 | A_13 |
| ATOM | 1151 | CA | LEU | 127 | 79.152 | 30.790 | 13.457 | 1.00 | 22.84 | A_13 |
| ATOM | 1152 | CB | LEU | 127 | 80.113 | 31.693 | 14.252 | 1.00 | 11.92 | A_13 |
| ATOM | 1153 | CG | LEU | 127 | 81.244 | 30.969 | 14.983 | 1.00 | 18.83 | A_13 |
| ATOM | 1154 | CD1 | LEU | 127 | 82.096 | 30.197 | 13.979 | 1.00 | 16.63 | A_13 |
| ATOM | 1155 | CD2 | LEU | 127 | 82.104 | 31.970 | 15.760 | 1.00 | 22.15 | A_13 |
| ATOM | 1156 | C | LEU | 127 | 77.802 | 30.699 | 14.163 | 1.00 | 21.02 | A_13 |
| ATOM | 1157 | O | LEU | 127 | 76.996 | 31.629 | 14.098 | 1.00 | 14.68 | A_13 |
| ATOM | 1158 | N | ASP | 128 | 77.563 | 29.572 | 14.828 | 1.00 | 18.87 | A_13 |
| ATOM | 1160 | CA | ASP | 128 | 76.336 | 29.345 | 15.571 | 1.00 | 16.46 | A_13 |
| ATOM | 1161 | CB | ASP | 128 | 75.996 | 27.855 | 15.540 | 1.00 | 17.60 | A_13 |
| ATOM | 1162 | CG | ASP | 128 | 74.577 | 27.552 | 15.996 | 1.00 | 23.55 | A_13 |
| ATOM | 1163 | OD1 | ASP | 128 | 73.796 | 28.488 | 16.258 | 1.00 | 10.00 | A_13 |
| ATOM | 1164 | OD2 | ASP | 128 | 74.236 | 26.355 | 16.087 | 1.00 | 32.36 | A_13 |
| ATOM | 1165 | C | ASP | 128 | 76.634 | 29.803 | 16.995 | 1.00 | 10.00 | A_13 |
| ATOM | 1166 | O | ASP | 128 | 77.650 | 30.420 | 17.244 | 1.00 | 29.54 | A_13 |
| ATOM | 1167 | N | HIS | 129 | 75.714 | 29.565 | 17.912 | 1.00 | 10.00 | A_13 |
| ATOM | 1169 | CA | HIS | 129 | 75.910 | 29.955 | 19.289 | 1.00 | 10.00 | A_13 |
| ATOM | 1170 | CB | HIS | 129 | 74.582 | 30.033 | 20.029 | 1.00 | 21.30 | A_13 |
| ATOM | 1171 | CG | HIS | 129 | 73.798 | 31.282 | 19.761 | 1.00 | 24.16 | A_13 |
| ATOM | 1172 | CD2 | HIS | 129 | 74.180 | 32.585 | 19.725 | 1.00 | 10.00 | A_13 |
| ATOM | 1173 | ND1 | HIS | 129 | 72.460 | 31.263 | 19.476 | 1.00 | 21.70 | A_13 |
| ATOM | 1175 | CE1 | HIS | 129 | 72.031 | 32.501 | 19.271 | 1.00 | 10.27 | A_13 |
| ATOM | 1176 | NE2 | HIS | 129 | 73.057 | 33.319 | 19.407 | 1.00 | 14.37 | A_13 |
| ATOM | 1177 | C | HIS | 129 | 76.780 | 28.947 | 19.992 | 1.00 | 30.04 | A_13 |
| ATOM | 1178 | O | HIS | 129 | 76.624 | 27.730 | 19.822 | 1.00 | 22.13 | A_13 |
| ATOM | 1179 | N | SER | 130 | 77.628 | 29.468 | 20.860 | 1.00 | 18.60 | A_13 |
| ATOM | 1181 | CA | SER | 130 | 78.534 | 28.662 | 21.636 | 1.00 | 10.79 | A_13 |
| ATOM | 1182 | CB | SER | 130 | 79.849 | 29.435 | 21.816 | 1.00 | 21.31 | A_13 |
| ATOM | 1183 | OG | SER | 130 | 80.782 | 28.731 | 22.616 | 1.00 | 16.34 | A_13 |
| ATOM | 1185 | C | SER | 130 | 77.898 | 28.368 | 22.987 | 1.00 | 31.13 | A_13 |
| ATOM | 1186 | O | SER | 130 | 76.962 | 29.060 | 23.440 | 1.00 | 15.87 | A_13 |
| ATOM | 1187 | N | LYS | 131 | 78.402 | 27.319 | 23.619 | 1.00 | 13.13 | A_13 |
| ATOM | 1189 | CA | LYS | 131 | 77.924 | 26.925 | 24.928 | 1.00 | 13.21 | A_13 |
| ATOM | 1190 | CB | LYS | 131 | 77.656 | 25.414 | 24.990 | 1.00 | 18.85 | A_13 |
| ATOM | 1191 | CG | LYS | 131 | 78.689 | 24.541 | 24.303 | 1.00 | 32.55 | A_13 |
| ATOM | 1192 | CD | LYS | 131 | 78.547 | 24.601 | 22.790 | 1.00 | 41.54 | A_13 |
| ATOM | 1193 | CE | LYS | 131 | 79.909 | 24.672 | 22.117 | 1.00 | 19.64 | A_13 |
| ATOM | 1194 | NZ | LYS | 131 | 80.747 | 25.799 | 22.617 | 1.00 | 13.47 | A_13 |
| ATOM | 1198 | C | LYS | 131 | 78.922 | 27.379 | 25.982 | 1.00 | 10.00 | A_13 |
| ATOM | 1199 | O | LYS | 131 | 78.666 | 27.260 | 27.185 | 1.00 | 13.35 | A_13 |
| ATOM | 1200 | N | ASP | 132 | 80.025 | 27.968 | 25.519 | 1.00 | 13.47 | A_13 |
| ATOM | 1202 | CA | ASP | 132 | 81.097 | 28.487 | 26.375 | 1.00 | 10.04 | A_13 |
| ATOM | 1203 | CB | ASP | 132 | 82.376 | 28.617 | 25.522 | 1.00 | 18.14 | A_13 |
| ATOM | 1204 | CG | ASP | 132 | 83.649 | 28.821 | 26.345 | 1.00 | 16.54 | A_13 |
| ATOM | 1205 | OD1 | ASP | 132 | 84.645 | 28.132 | 26.028 | 1.00 | 36.08 | A_13 |

50/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1206 | OD2 | ASP | 132 | 83.685 | 29.660 | 27.276 | 1.00 | 15.60 | A_13 |
| ATOM | 1207 | C | ASP | 132 | 80.603 | 29.875 | 26.836 | 1.00 | 18.74 | A_13 |
| ATOM | 1208 | O | ASP | 132 | 80.559 | 30.816 | 26.038 | 1.00 | 14.61 | A_13 |
| ATOM | 1209 | N | PRO | 133 | 80.305 | 30.039 | 28.142 | 1.00 | 15.61 | A_13 |
| ATOM | 1210 | CD | PRO | 133 | 80.617 | 29.127 | 29.251 | 1.00 | 21.19 | A_13 |
| ATOM | 1211 | CA | PRO | 133 | 79.818 | 31.320 | 28.662 | 1.00 | 10.00 | A_13 |
| ATOM | 1212 | CB | PRO | 133 | 79.542 | 31.007 | 30.135 | 1.00 | 10.00 | A_13 |
| ATOM | 1213 | CG | PRO | 133 | 80.633 | 30.063 | 30.450 | 1.00 | 30.94 | A_13 |
| ATOM | 1214 | C | PRO | 133 | 80.834 | 32.444 | 28.511 | 1.00 | 22.87 | A_13 |
| ATOM | 1215 | O | PRO | 133 | 80.526 | 33.574 | 28.742 | 1.00 | 21.65 | A_13 |
| ATOM | 1216 | N | GLY | 134 | 82.070 | 32.115 | 28.174 | 1.00 | 20.95 | A_13 |
| ATOM | 1218 | CA | GLY | 134 | 83.055 | 33.167 | 28.028 | 1.00 | 15.22 | A_13 |
| ATOM | 1219 | C | GLY | 134 | 83.182 | 33.578 | 26.581 | 1.00 | 34.54 | A_13 |
| ATOM | 1220 | O | GLY | 134 | 83.962 | 34.488 | 26.252 | 1.00 | 18.06 | A_13 |
| ATOM | 1221 | N | ALA | 135 | 82.490 | 32.846 | 25.706 | 1.00 | 21.09 | A_13 |
| ATOM | 1223 | CA | ALA | 135 | 82.547 | 33.110 | 24.263 | 1.00 | 27.50 | A_13 |
| ATOM | 1224 | CB | ALA | 135 | 82.131 | 31.858 | 23.453 | 1.00 | 10.00 | A_13 |
| ATOM | 1225 | C | ALA | 135 | 81.722 | 34.308 | 23.814 | 1.00 | 21.74 | A_13 |
| ATOM | 1226 | O | ALA | 135 | 80.641 | 34.556 | 24.328 | 1.00 | 13.84 | A_13 |
| ATOM | 1227 | N | LEU | 136 | 82.220 | 34.990 | 22.787 | 1.00 | 19.10 | A_13 |
| ATOM | 1229 | CA | LEU | 136 | 81.540 | 36.140 | 22.203 | 1.00 | 21.65 | A_13 |
| ATOM | 1230 | CB | LEU | 136 | 82.448 | 36.803 | 21.161 | 1.00 | 10.00 | A_13 |
| ATOM | 1231 | CG | LEU | 136 | 81.964 | 37.898 | 20.201 | 1.00 | 17.22 | A_13 |
| ATOM | 1232 | CD1 | LEU | 136 | 81.250 | 37.296 | 19.024 | 1.00 | 24.18 | A_13 |
| ATOM | 1233 | CD2 | LEU | 136 | 81.113 | 38.896 | 20.905 | 1.00 | 10.00 | A_13 |
| ATOM | 1234 | C | LEU | 136 | 80.250 | 35.632 | 21.558 | 1.00 | 19.32 | A_13 |
| ATOM | 1235 | O | LEU | 136 | 79.266 | 36.359 | 21.458 | 1.00 | 26.20 | A_13 |
| ATOM | 1236 | N | MET | 137 | 80.297 | 34.409 | 21.029 | 1.00 | 10.00 | A_13 |
| ATOM | 1238 | CA | MET | 137 | 79.123 | 33.791 | 20.423 | 1.00 | 10.02 | A_13 |
| ATOM | 1239 | CB | MET | 137 | 79.507 | 32.691 | 19.428 | 1.00 | 15.14 | A_13 |
| ATOM | 1240 | CG | MET | 137 | 80.181 | 33.223 | 18.169 | 1.00 | 16.42 | A_13 |
| ATOM | 1241 | SD | MET | 137 | 79.366 | 34.665 | 17.397 | 1.00 | 10.65 | A_13 |
| ATOM | 1242 | CE | MET | 137 | 77.848 | 34.005 | 16.975 | 1.00 | 10.87 | A_13 |
| ATOM | 1243 | C | MET | 137 | 78.122 | 33.256 | 21.447 | 1.00 | 12.70 | A_13 |
| ATOM | 1244 | O | MET | 137 | 77.187 | 32.539 | 21.087 | 1.00 | 10.00 | A_13 |
| ATOM | 1245 | N | PHE | 138 | 78.295 | 33.627 | 22.713 | 1.00 | 18.70 | A_13 |
| ATOM | 1247 | CA | PHE | 138 | 77.370 | 33.196 | 23.759 | 1.00 | 24.08 | A_13 |
| ATOM | 1248 | CB | PHE | 138 | 77.954 | 33.448 | 25.159 | 1.00 | 24.15 | A_13 |
| ATOM | 1249 | CG | PHE | 138 | 77.306 | 32.617 | 26.240 | 1.00 | 29.38 | A_13 |
| ATOM | 1250 | CD1 | PHE | 138 | 76.694 | 33.222 | 27.336 | 1.00 | 27.07 | A_13 |
| ATOM | 1251 | CD2 | PHE | 138 | 77.253 | 31.226 | 26.123 | 1.00 | 21.37 | A_13 |
| ATOM | 1252 | CE1 | PHE | 138 | 76.033 | 32.455 | 28.289 | 1.00 | 30.35 | A_13 |
| ATOM | 1253 | CE2 | PHE | 138 | 76.599 | 30.458 | 27.065 | 1.00 | 19.58 | A_13 |
| ATOM | 1254 | CZ | PHE | 138 | 75.986 | 31.070 | 28.154 | 1.00 | 17.69 | A_13 |
| ATOM | 1255 | C | PHE | 138 | 76.074 | 33.992 | 23.513 | 1.00 | 14.20 | A_13 |
| ATOM | 1256 | O | PHE | 138 | 76.115 | 35.105 | 23.014 | 1.00 | 10.27 | A_13 |
| ATOM | 1257 | N | PRO | 139 | 74.899 | 33.366 | 23.730 | 1.00 | 13.04 | A_13 |
| ATOM | 1258 | CD | PRO | 139 | 74.664 | 31.975 | 24.131 | 1.00 | 11.17 | A_13 |
| ATOM | 1259 | CA | PRO | 139 | 73.619 | 34.043 | 23.504 | 1.00 | 18.27 | A_13 |
| ATOM | 1260 | CB | PRO | 139 | 72.625 | 32.875 | 23.384 | 1.00 | 14.33 | A_13 |
| ATOM | 1261 | CG | PRO | 139 | 73.474 | 31.634 | 23.305 | 1.00 | 24.22 | A_13 |
| ATOM | 1262 | C | PRO | 139 | 73.162 | 35.018 | 24.584 | 1.00 | 16.51 | A_13 |
| ATOM | 1263 | O | PRO | 139 | 72.023 | 35.467 | 24.535 | 1.00 | 24.45 | A_13 |
| ATOM | 1264 | N | ILE | 140 | 74.034 | 35.375 | 25.524 | 1.00 | 23.16 | A_13 |
| ATOM | 1266 | CA | ILE | 140 | 73.652 | 36.290 | 26.604 | 1.00 | 25.00 | A_13 |
| ATOM | 1267 | CB | ILE | 140 | 73.688 | 35.559 | 27.966 | 1.00 | 12.10 | A_13 |
| ATOM | 1268 | CG2 | ILE | 140 | 73.336 | 36.519 | 29.085 | 1.00 | 12.62 | A_13 |
| ATOM | 1269 | CG1 | ILE | 140 | 72.738 | 34.341 | 27.904 | 1.00 | 22.67 | A_13 |
| ATOM | 1270 | CD1 | ILE | 140 | 72.827 | 33.353 | 29.073 | 1.00 | 27.73 | A_13 |
| ATOM | 1271 | C | ILE | 140 | 74.584 | 37.489 | 26.621 | 1.00 | 30.64 | A_13 |
| ATOM | 1272 | O | ILE | 140 | 75.778 | 37.317 | 26.682 | 1.00 | 23.16 | A_13 |
| ATOM | 1273 | N | TYR | 141 | 74.033 | 38.694 | 26.532 | 1.00 | 21.05 | A_13 |
| ATOM | 1275 | CA | TYR | 141 | 74.851 | 39.901 | 26.528 | 1.00 | 20.10 | A_13 |
| ATOM | 1276 | CB | TYR | 141 | 74.017 | 41.122 | 26.129 | 1.00 | 17.66 | A_13 |
| ATOM | 1277 | CG | TYR | 141 | 74.784 | 42.433 | 26.103 | 1.00 | 22.24 | A_13 |
| ATOM | 1278 | CD1 | TYR | 141 | 74.711 | 43.318 | 27.171 | 1.00 | 18.07 | A_13 |
| ATOM | 1279 | CE1 | TYR | 141 | 75.386 | 44.527 | 27.144 | 1.00 | 19.84 | A_13 |
| ATOM | 1280 | CD2 | TYR | 141 | 75.563 | 42.798 | 24.999 | 1.00 | 18.08 | A_13 |
| ATOM | 1281 | CE2 | TYR | 141 | 76.244 | 44.008 | 24.961 | 1.00 | 10.00 | A_13 |
| ATOM | 1282 | CZ | TYR | 141 | 76.149 | 44.867 | 26.038 | 1.00 | 25.17 | A_13 |
| ATOM | 1283 | OH | TYR | 141 | 76.814 | 46.070 | 26.043 | 1.00 | 30.78 | A_13 |
| ATOM | 1285 | C | TYR | 141 | 75.533 | 40.169 | 27.852 | 1.00 | 19.61 | A_13 |
| ATOM | 1286 | O | TYR | 141 | 74.910 | 40.146 | 28.913 | 1.00 | 16.08 | A_13 |
| ATOM | 1287 | N | THR | 142 | 76.817 | 40.476 | 27.772 | 1.00 | 26.26 | A_13 |
| ATOM | 1289 | CA | THR | 142 | 77.612 | 40.788 | 28.944 | 1.00 | 24.52 | A_13 |
| ATOM | 1290 | CB | THR | 142 | 78.498 | 39.568 | 29.362 | 1.00 | 10.00 | A_13 |
| ATOM | 1291 | OG1 | THR | 142 | 77.664 | 38.587 | 29.981 | 1.00 | 37.30 | A_13 |

51/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1293 | CG2 | THR | 142 | 79.543 | 39.961 | 30.390 | 1.00 | 14.88 | A_13 |
| ATOM | 1294 | C | THR | 142 | 78.467 | 41.976 | 28.580 | 1.00 | 25.46 | A_13 |
| ATOM | 1295 | O | THR | 142 | 78.980 | 42.058 | 27.464 | 1.00 | 10.00 | A_13 |
| ATOM | 1296 | N | TYR | 143 | 78.575 | 42.947 | 29.476 | 1.00 | 20.23 | A_13 |
| ATOM | 1298 | CA | TYR | 143 | 79.412 | 44.079 | 29.133 | 1.00 | 32.69 | A_13 |
| ATOM | 1299 | CB | TYR | 143 | 79.024 | 45.363 | 29.854 | 1.00 | 35.01 | A_13 |
| ATOM | 1300 | CG | TYR | 143 | 79.834 | 46.531 | 29.347 | 1.00 | 16.01 | A_13 |
| ATOM | 1301 | CD1 | TYR | 143 | 79.776 | 46.910 | 27.998 | 1.00 | 12.56 | A_13 |
| ATOM | 1302 | CE1 | TYR | 143 | 80.554 | 47.961 | 27.510 | 1.00 | 19.23 | A_13 |
| ATOM | 1303 | CD2 | TYR | 143 | 80.690 | 47.230 | 30.196 | 1.00 | 19.43 | A_13 |
| ATOM | 1304 | CE2 | TYR | 143 | 81.478 | 48.287 | 29.719 | 1.00 | 15.52 | A_13 |
| ATOM | 1305 | CZ | TYR | 143 | 81.403 | 48.643 | 28.376 | 1.00 | 12.56 | A_13 |
| ATOM | 1306 | OH | TYR | 143 | 82.193 | 49.654 | 27.892 | 1.00 | 18.85 | A_13 |
| ATOM | 1308 | C | TYR | 143 | 80.871 | 43.754 | 29.382 | 1.00 | 25.10 | A_13 |
| ATOM | 1309 | O | TYR | 143 | 81.373 | 43.846 | 30.503 | 1.00 | 28.90 | A_13 |
| ATOM | 1310 | N | THR | 144 | 81.539 | 43.375 | 28.303 | 1.00 | 35.25 | A_13 |
| ATOM | 1312 | CA | THR | 144 | 82.946 | 43.029 | 28.336 | 1.00 | 38.86 | A_13 |
| ATOM | 1313 | CB | THR | 144 | 83.158 | 41.568 | 27.873 | 1.00 | 23.22 | A_13 |
| ATOM | 1314 | OG1 | THR | 144 | 82.129 | 41.219 | 26.934 | 1.00 | 35.22 | A_13 |
| ATOM | 1316 | CG2 | THR | 144 | 83.105 | 40.616 | 29.082 | 1.00 | 17.53 | A_13 |
| ATOM | 1317 | C | THR | 144 | 83.720 | 44.017 | 27.488 | 1.00 | 21.63 | A_13 |
| ATOM | 1318 | O | THR | 144 | 84.434 | 43.651 | 26.556 | 1.00 | 37.44 | A_13 |
| ATOM | 1319 | N | GLY | 145 | 83.504 | 45.288 | 27.798 | 1.00 | 14.47 | A_13 |
| ATOM | 1321 | CA | GLY | 145 | 84.200 | 46.375 | 27.131 | 1.00 | 24.39 | A_13 |
| ATOM | 1322 | C | GLY | 145 | 84.119 | 46.536 | 25.628 | 1.00 | 41.65 | A_13 |
| ATOM | 1323 | O | GLY | 145 | 84.053 | 45.565 | 24.877 | 1.00 | 42.39 | A_13 |
| ATOM | 1324 | N | LYS | 146 | 84.122 | 47.792 | 25.195 | 1.00 | 33.04 | A_13 |
| ATOM | 1326 | CA | LYS | 146 | 84.059 | 48.103 | 23.778 | 1.00 | 29.29 | A_13 |
| ATOM | 1327 | CB | LYS | 146 | 83.260 | 49.392 | 23.539 | 1.00 | 26.47 | A_13 |
| ATOM | 1328 | CG | LYS | 146 | 83.087 | 49.721 | 22.059 | 1.00 | 33.24 | A_13 |
| ATOM | 1329 | CD | LYS | 146 | 82.812 | 51.194 | 21.833 | 1.00 | 13.70 | A_13 |
| ATOM | 1330 | CE | LYS | 146 | 82.620 | 51.497 | 20.343 | 1.00 | 18.35 | A_13 |
| ATOM | 1331 | NZ | LYS | 146 | 83.766 | 51.122 | 19.477 | 1.00 | 30.66 | A_13 |
| ATOM | 1335 | C | LYS | 146 | 85.491 | 48.297 | 23.308 | 1.00 | 41.61 | A_13 |
| ATOM | 1336 | O | LYS | 146 | 86.028 | 49.412 | 23.382 | 1.00 | 46.44 | A_13 |
| ATOM | 1337 | N | SER | 147 | 86.130 | 47.206 | 22.898 | 1.00 | 34.67 | A_13 |
| ATOM | 1339 | CA | SER | 147 | 87.509 | 47.258 | 22.416 | 1.00 | 30.76 | A_13 |
| ATOM | 1340 | CB | SER | 147 | 87.624 | 48.258 | 21.249 | 1.00 | 24.56 | A_13 |
| ATOM | 1341 | OG | SER | 147 | 86.638 | 48.002 | 20.257 | 1.00 | 31.81 | A_13 |
| ATOM | 1343 | C | SER | 147 | 88.464 | 47.626 | 23.567 | 1.00 | 33.60 | A_13 |
| ATOM | 1344 | O | SER | 147 | 88.789 | 48.806 | 23.789 | 1.00 | 39.96 | A_13 |
| ATOM | 1345 | N | HIS | 148 | 88.862 | 46.611 | 24.331 | 1.00 | 36.71 | A_13 |
| ATOM | 1347 | CA | HIS | 148 | 89.778 | 46.769 | 25.467 | 1.00 | 34.40 | A_13 |
| ATOM | 1348 | CB | HIS | 148 | 89.307 | 47.862 | 26.438 | 1.00 | 26.40 | A_13 |
| ATOM | 1349 | CG | HIS | 148 | 90.251 | 49.022 | 26.537 | 1.00 | 39.11 | A_13 |
| ATOM | 1350 | CD2 | HIS | 148 | 90.929 | 49.542 | 27.588 | 1.00 | 30.52 | A_13 |
| ATOM | 1351 | ND1 | HIS | 148 | 90.635 | 49.767 | 25.437 | 1.00 | 37.71 | A_13 |
| ATOM | 1353 | CE1 | HIS | 148 | 91.511 | 50.681 | 25.807 | 1.00 | 29.04 | A_13 |
| ATOM | 1354 | NE2 | HIS | 148 | 91.707 | 50.567 | 27.110 | 1.00 | 29.03 | A_13 |
| ATOM | 1356 | C | HIS | 148 | 89.949 | 45.436 | 26.190 | 1.00 | 39.41 | A_13 |
| ATOM | 1357 | O | HIS | 148 | 90.134 | 45.373 | 27.411 | 1.00 | 35.01 | A_13 |
| ATOM | 1358 | N | PHE | 149 | 89.840 | 44.386 | 25.383 | 1.00 | 25.35 | A_13 |
| ATOM | 1360 | CA | PHE | 149 | 89.996 | 42.966 | 25.721 | 1.00 | 30.54 | A_13 |
| ATOM | 1361 | CB | PHE | 149 | 88.788 | 42.423 | 26.495 | 1.00 | 33.34 | A_13 |
| ATOM | 1362 | CG | PHE | 149 | 88.951 | 42.440 | 27.996 | 1.00 | 31.37 | A_13 |
| ATOM | 1363 | CD1 | PHE | 149 | 89.387 | 41.302 | 28.673 | 1.00 | 30.46 | A_13 |
| ATOM | 1364 | CD2 | PHE | 149 | 88.624 | 43.575 | 28.740 | 1.00 | 40.67 | A_13 |
| ATOM | 1365 | CE1 | PHE | 149 | 89.492 | 41.293 | 30.075 | 1.00 | 18.92 | A_13 |
| ATOM | 1366 | CE2 | PHE | 149 | 88.728 | 43.574 | 30.136 | 1.00 | 23.23 | A_13 |
| ATOM | 1367 | CZ | PHE | 149 | 89.161 | 42.430 | 30.803 | 1.00 | 17.03 | A_13 |
| ATOM | 1368 | C | PHE | 149 | 90.026 | 42.366 | 24.295 | 1.00 | 41.76 | A_13 |
| ATOM | 1369 | O | PHE | 149 | 89.967 | 43.119 | 23.307 | 1.00 | 40.43 | A_13 |
| ATOM | 1370 | N | MET | 150 | 90.132 | 41.050 | 24.142 | 1.00 | 31.30 | A_13 |
| ATOM | 1372 | CA | MET | 150 | 90.152 | 40.531 | 22.779 | 1.00 | 20.65 | A_13 |
| ATOM | 1373 | CB | MET | 150 | 91.588 | 40.195 | 22.352 | 1.00 | 28.29 | A_13 |
| ATOM | 1374 | CG | MET | 150 | 92.494 | 41.436 | 22.188 | 1.00 | 34.71 | A_13 |
| ATOM | 1375 | SD | MET | 150 | 91.750 | 42.780 | 21.185 | 1.00 | 67.91 | A_13 |
| ATOM | 1376 | CE | MET | 150 | 92.512 | 42.498 | 19.518 | 1.00 | 22.43 | A_13 |
| ATOM | 1377 | C | MET | 150 | 89.201 | 39.370 | 22.497 | 1.00 | 21.51 | A_13 |
| ATOM | 1378 | O | MET | 150 | 88.498 | 38.901 | 23.391 | 1.00 | 25.37 | A_13 |
| ATOM | 1379 | N | LEU | 151 | 89.159 | 38.938 | 21.240 | 1.00 | 13.78 | A_13 |
| ATOM | 1381 | CA | LEU | 151 | 88.313 | 37.825 | 20.834 | 1.00 | 14.73 | A_13 |
| ATOM | 1382 | CB | LEU | 151 | 88.435 | 37.589 | 19.321 | 1.00 | 15.49 | A_13 |
| ATOM | 1383 | CG | LEU | 151 | 87.535 | 36.511 | 18.691 | 1.00 | 27.05 | A_13 |
| ATOM | 1384 | CD1 | LEU | 151 | 86.070 | 36.915 | 18.847 | 1.00 | 10.98 | A_13 |
| ATOM | 1385 | CD2 | LEU | 151 | 87.879 | 36.310 | 17.208 | 1.00 | 15.73 | A_13 |
| ATOM | 1386 | C | LEU | 151 | 88.732 | 36.563 | 21.600 | 1.00 | 25.01 | A_13 |

52/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1387 | O | LEU | 151 | 89.912 | 36.178 | 21.589 | 1.00 | 17.37 | A_13 |
| ATOM | 1388 | N | PRO | 152 | 87.777 | 35.927 | 22.306 | 1.00 | 10.37 | A_13 |
| ATOM | 1389 | CD | PRO | 152 | 86.425 | 36.450 | 22.575 | 1.00 | 15.35 | A_13 |
| ATOM | 1390 | CA | PRO | 152 | 88.030 | 34.712 | 23.087 | 1.00 | 11.49 | A_13 |
| ATOM | 1391 | CB | PRO | 152 | 86.658 | 34.412 | 23.702 | 1.00 | 15.98 | A_13 |
| ATOM | 1392 | CG | PRO | 152 | 86.083 | 35.789 | 23.898 | 1.00 | 27.60 | A_13 |
| ATOM | 1393 | C | PRO | 152 | 88.533 | 33.553 | 22.230 | 1.00 | 18.06 | A_13 |
| ATOM | 1394 | O | PRO | 152 | 88.160 | 33.430 | 21.063 | 1.00 | 16.21 | A_13 |
| ATOM | 1395 | N | ASP | 153 | 89.350 | 32.696 | 22.836 | 1.00 | 15.86 | A_13 |
| ATOM | 1397 | CA | ASP | 153 | 89.933 | 31.526 | 22.185 | 1.00 | 20.25 | A_13 |
| ATOM | 1398 | CB | ASP | 153 | 90.632 | 30.630 | 23.227 | 1.00 | 18.17 | A_13 |
| ATOM | 1399 | CG | ASP | 153 | 91.843 | 31.301 | 23.908 | 1.00 | 24.01 | A_13 |
| ATOM | 1400 | OD1 | ASP | 153 | 92.517 | 32.159 | 23.284 | 1.00 | 14.96 | A_13 |
| ATOM | 1401 | OD2 | ASP | 153 | 92.131 | 30.937 | 25.077 | 1.00 | 20.20 | A_13 |
| ATOM | 1402 | C | ASP | 153 | 88.887 | 30.678 | 21.452 | 1.00 | 24.64 | A_13 |
| ATOM | 1403 | O | ASP | 153 | 89.113 | 30.221 | 20.330 | 1.00 | 13.51 | A_13 |
| ATOM | 1404 | N | ASP | 154 | 87.757 | 30.453 | 22.114 | 1.00 | 24.11 | A_13 |
| ATOM | 1406 | CA | ASP | 154 | 86.664 | 29.657 | 21.577 | 1.00 | 19.19 | A_13 |
| ATOM | 1407 | CB | ASP | 154 | 85.527 | 29.632 | 22.587 | 1.00 | 18.27 | A_13 |
| ATOM | 1408 | CG | ASP | 154 | 84.406 | 28.751 | 22.161 | 1.00 | 24.26 | A_13 |
| ATOM | 1409 | OD1 | ASP | 154 | 83.314 | 29.291 | 21.950 | 1.00 | 20.97 | A_13 |
| ATOM | 1410 | OD2 | ASP | 154 | 84.609 | 27.530 | 22.031 | 1.00 | 20.32 | A_13 |
| ATOM | 1411 | C | ASP | 154 | 86.162 | 30.170 | 20.229 | 1.00 | 18.99 | A_13 |
| ATOM | 1412 | O | ASP | 154 | 86.043 | 29.408 | 19.277 | 1.00 | 22.56 | A_13 |
| ATOM | 1413 | N | ASP | 155 | 85.873 | 31.465 | 20.158 | 1.00 | 16.11 | A_13 |
| ATOM | 1415 | CA | ASP | 155 | 85.407 | 32.078 | 18.917 | 1.00 | 25.30 | A_13 |
| ATOM | 1416 | CB | ASP | 155 | 85.011 | 33.527 | 19.158 | 1.00 | 13.32 | A_13 |
| ATOM | 1417 | CG | ASP | 155 | 83.975 | 33.655 | 20.249 | 1.00 | 11.19 | A_13 |
| ATOM | 1418 | OD1 | ASP | 155 | 84.347 | 34.136 | 21.332 | 1.00 | 12.26 | A_13 |
| ATOM | 1419 | OD2 | ASP | 155 | 82.810 | 33.255 | 20.029 | 1.00 | 10.00 | A_13 |
| ATOM | 1420 | C | ASP | 155 | 86.461 | 31.992 | 17.828 | 1.00 | 13.98 | A_13 |
| ATOM | 1421 | O | ASP | 155 | 86.141 | 31.656 | 16.687 | 1.00 | 14.08 | A_13 |
| ATOM | 1422 | N | VAL | 156 | 87.713 | 32.310 | 18.160 | 1.00 | 16.49 | A_13 |
| ATOM | 1424 | CA | VAL | 156 | 88.771 | 32.201 | 17.159 | 1.00 | 27.34 | A_13 |
| ATOM | 1425 | CB | VAL | 156 | 90.145 | 32.826 | 17.625 | 1.00 | 23.59 | A_13 |
| ATOM | 1426 | CG1 | VAL | 156 | 90.327 | 32.750 | 19.119 | 1.00 | 13.94 | A_13 |
| ATOM | 1427 | CG2 | VAL | 156 | 91.312 | 32.153 | 16.919 | 1.00 | 21.70 | A_13 |
| ATOM | 1428 | C | VAL | 156 | 88.874 | 30.738 | 16.657 | 1.00 | 16.95 | A_13 |
| ATOM | 1429 | O | VAL | 156 | 88.946 | 30.506 | 15.448 | 1.00 | 13.79 | A_13 |
| ATOM | 1430 | N | GLN | 157 | 88.762 | 29.763 | 17.561 | 1.00 | 19.45 | A_13 |
| ATOM | 1432 | CA | GLN | 157 | 88.796 | 28.352 | 17.154 | 1.00 | 30.53 | A_13 |
| ATOM | 1433 | CB | GLN | 157 | 88.579 | 27.422 | 18.353 | 1.00 | 23.08 | A_13 |
| ATOM | 1434 | CG | GLN | 157 | 89.633 | 27.521 | 19.452 | 1.00 | 24.83 | A_13 |
| ATOM | 1435 | CD | GLN | 157 | 90.950 | 26.872 | 19.089 | 1.00 | 20.26 | A_13 |
| ATOM | 1436 | OE1 | GLN | 157 | 91.743 | 27.422 | 18.316 | 1.00 | 25.80 | A_13 |
| ATOM | 1437 | NE2 | GLN | 157 | 91.204 | 25.702 | 19.673 | 1.00 | 38.67 | A_13 |
| ATOM | 1440 | C | GLN | 157 | 87.667 | 28.136 | 16.148 | 1.00 | 14.16 | A_13 |
| ATOM | 1441 | O | GLN | 157 | 87.869 | 27.541 | 15.096 | 1.00 | 14.11 | A_13 |
| ATOM | 1442 | N | GLY | 158 | 86.505 | 28.709 | 16.437 | 1.00 | 19.16 | A_13 |
| ATOM | 1444 | CA | GLY | 158 | 85.361 | 28.584 | 15.551 | 1.00 | 12.79 | A_13 |
| ATOM | 1445 | C | GLY | 158 | 85.510 | 29.144 | 14.143 | 1.00 | 24.46 | A_13 |
| ATOM | 1446 | O | GLY | 158 | 85.181 | 28.449 | 13.177 | 1.00 | 18.77 | A_13 |
| ATOM | 1447 | N | ILE | 159 | 85.936 | 30.403 | 13.989 | 1.00 | 22.41 | A_13 |
| ATOM | 1449 | CA | ILE | 159 | 86.091 | 30.946 | 12.628 | 1.00 | 31.18 | A_13 |
| ATOM | 1450 | CB | ILE | 159 | 86.300 | 32.508 | 12.532 | 1.00 | 23.53 | A_13 |
| ATOM | 1451 | CG2 | ILE | 159 | 84.991 | 33.203 | 12.177 | 1.00 | 17.28 | A_13 |
| ATOM | 1452 | CG1 | ILE | 159 | 87.022 | 33.063 | 13.758 | 1.00 | 15.28 | A_13 |
| ATOM | 1453 | CD1 | ILE | 159 | 88.507 | 32.949 | 13.707 | 1.00 | 14.71 | A_13 |
| ATOM | 1454 | C | ILE | 159 | 87.226 | 30.280 | 11.875 | 1.00 | 10.56 | A_13 |
| ATOM | 1455 | O | ILE | 159 | 87.167 | 30.139 | 10.653 | 1.00 | 18.79 | A_13 |
| ATOM | 1456 | N | GLN | 160 | 88.287 | 29.927 | 12.590 | 1.00 | 20.71 | A_13 |
| ATOM | 1458 | CA | GLN | 160 | 89.411 | 29.294 | 11.943 | 1.00 | 10.00 | A_13 |
| ATOM | 1459 | CB | GLN | 160 | 90.640 | 29.274 | 12.855 | 1.00 | 10.00 | A_13 |
| ATOM | 1460 | CG | GLN | 160 | 91.114 | 30.690 | 13.182 | 1.00 | 13.93 | A_13 |
| ATOM | 1461 | CD | GLN | 160 | 92.402 | 30.754 | 13.981 | 1.00 | 25.61 | A_13 |
| ATOM | 1462 | OE1 | GLN | 160 | 92.814 | 29.786 | 14.629 | 1.00 | 19.40 | A_13 |
| ATOM | 1463 | NE2 | GLN | 160 | 93.042 | 31.915 | 13.950 | 1.00 | 24.78 | A_13 |
| ATOM | 1466 | C | GLN | 160 | 89.000 | 27.917 | 11.477 | 1.00 | 10.00 | A_13 |
| ATOM | 1467 | O | GLN | 160 | 89.458 | 27.481 | 10.432 | 1.00 | 21.73 | A_13 |
| ATOM | 1468 | N | SER | 161 | 88.068 | 27.268 | 12.186 | 1.00 | 10.00 | A_13 |
| ATOM | 1470 | CA | SER | 161 | 87.610 | 25.946 | 11.760 | 1.00 | 11.63 | A_13 |
| ATOM | 1471 | CB | SER | 161 | 86.688 | 25.292 | 12.800 | 1.00 | 18.40 | A_13 |
| ATOM | 1472 | OG | SER | 161 | 85.365 | 25.795 | 12.759 | 1.00 | 15.44 | A_13 |
| ATOM | 1474 | C | SER | 161 | 86.913 | 26.048 | 10.396 | 1.00 | 26.18 | A_13 |
| ATOM | 1475 | O | SER | 161 | 86.839 | 25.065 | 9.654 | 1.00 | 13.96 | A_13 |
| ATOM | 1476 | N | LEU | 162 | 86.428 | 27.247 | 10.070 | 1.00 | 19.36 | A_13 |
| ATOM | 1478 | CA | LEU | 162 | 85.749 | 27.493 | 8.808 | 1.00 | 17.21 | A_13 |

53/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1479 | CB | LEU | 162 | 84.584 | 28.477 | 9.007 | 1.00 | 14.37 | A_13 |
| ATOM | 1480 | CG | LEU | 162 | 83.489 | 28.144 | 10.021 | 1.00 | 31.09 | A_13 |
| ATOM | 1481 | CD1 | LEU | 162 | 82.596 | 29.351 | 10.217 | 1.00 | 14.96 | A_13 |
| ATOM | 1482 | CD2 | LEU | 162 | 82.672 | 26.949 | 9.548 | 1.00 | 23.87 | A_13 |
| ATOM | 1483 | C | LEU | 162 | 86.654 | 28.080 | 7.744 | 1.00 | 11.98 | A_13 |
| ATOM | 1484 | O | LEU | 162 | 86.596 | 27.680 | 6.584 | 1.00 | 15.25 | A_13 |
| ATOM | 1485 | N | TYR | 163 | 87.459 | 29.063 | 8.135 | 1.00 | 26.64 | A_13 |
| ATOM | 1487 | CA | TYR | 163 | 88.320 | 29.796 | 7.204 | 1.00 | 18.28 | A_13 |
| ATOM | 1488 | CB | TYR | 163 | 87.977 | 31.289 | 7.277 | 1.00 | 26.89 | A_13 |
| ATOM | 1489 | CG | TYR | 163 | 86.519 | 31.600 | 7.039 | 1.00 | 18.80 | A_13 |
| ATOM | 1490 | CD1 | TYR | 163 | 86.027 | 31.744 | 5.749 | 1.00 | 10.00 | A_13 |
| ATOM | 1491 | CE1 | TYR | 163 | 84.680 | 31.936 | 5.515 | 1.00 | 12.83 | A_13 |
| ATOM | 1492 | CD2 | TYR | 163 | 85.622 | 31.672 | 8.099 | 1.00 | 16.58 | A_13 |
| ATOM | 1493 | CE2 | TYR | 163 | 84.266 | 31.867 | 7.873 | 1.00 | 12.32 | A_13 |
| ATOM | 1494 | CZ | TYR | 163 | 83.807 | 31.991 | 6.576 | 1.00 | 11.77 | A_13 |
| ATOM | 1495 | OH | TYR | 163 | 82.472 | 32.141 | 6.331 | 1.00 | 21.93 | A_13 |
| ATOM | 1497 | C | TYR | 163 | 89.818 | 29.669 | 7.397 | 1.00 | 15.67 | A_13 |
| ATOM | 1498 | O | TYR | 163 | 90.590 | 30.089 | 6.526 | 1.00 | 18.92 | A_13 |
| ATOM | 1499 | N | GLY | 164 | 90.225 | 29.096 | 8.525 | 1.00 | 18.34 | A_13 |
| ATOM | 1501 | CA | GLY | 164 | 91.636 | 28.966 | 8.826 | 1.00 | 10.61 | A_13 |
| ATOM | 1502 | C | GLY | 164 | 92.149 | 30.215 | 9.525 | 1.00 | 15.63 | A_13 |
| ATOM | 1503 | O | GLY | 164 | 91.334 | 31.139 | 9.775 | 1.00 | 21.42 | A_13 |
| ATOM | 1504 | OT | GLY | 164 | 93.353 | 30.250 | 9.858 | 1.00 | 21.99 | A_13 |
| ATOM | 3009 | ZN | ZN | 166 | 73.275 | 35.223 | 18.371 | 1.00 | 27.40 | AION |
| ATOM | 3010 | ZN | ZN | 167 | 65.511 | 41.122 | 10.564 | 1.00 | 27.86 | AION |
| ATOM | 3011 | CA | CA | 168 | 64.285 | 44.152 | 21.635 | 1.00 | 11.76 | AION |
| ATOM | 3012 | CA | CA | 165 | 73.319 | 39.377 | 1.854 | 1.00 | 40.73 | AION |
| ATOM | 3017 | C5 | WAY | 169 | 67.400 | 35.999 | 20.267 | 1.00 | 38.86 | A693 |
| ATOM | 3018 | CF1 | WAY | 169 | 66.626 | 35.606 | 19.161 | 1.00 | 30.96 | A693 |
| ATOM | 3019 | CH | WAY | 169 | 67.199 | 35.400 | 17.901 | 1.00 | 41.17 | A693 |
| ATOM | 3020 | C2 | WAY | 169 | 68.561 | 35.623 | 17.728 | 1.00 | 36.26 | A693 |
| ATOM | 3021 | C3 | WAY | 169 | 69.339 | 36.039 | 18.811 | 1.00 | 35.73 | A693 |
| ATOM | 3022 | C4 | WAY | 169 | 68.807 | 36.216 | 20.078 | 1.00 | 33.71 | A693 |
| ATOM | 3023 | N20 | WAY | 169 | 69.699 | 36.617 | 21.141 | 1.00 | 33.16 | A693 |
| ATOM | 3024 | CD | WAY | 169 | 70.137 | 35.640 | 22.189 | 1.00 | 29.78 | A693 |
| ATOM | 3025 | C23 | WAY | 169 | 68.986 | 34.739 | 22.685 | 1.00 | 25.69 | A693 |
| ATOM | 3026 | C28 | WAY | 169 | 68.187 | 35.088 | 23.798 | 1.00 | 31.72 | A693 |
| ATOM | 3027 | C27 | WAY | 169 | 67.141 | 34.238 | 24.205 | 1.00 | 33.61 | A693 |
| ATOM | 3028 | CM | WAY | 169 | 66.921 | 33.061 | 23.490 | 1.00 | 32.16 | A693 |
| ATOM | 3029 | N25 | WAY | 169 | 67.703 | 32.748 | 22.426 | 1.00 | 42.39 | A693 |
| ATOM | 3030 | C24 | WAY | 169 | 68.709 | 33.546 | 22.016 | 1.00 | 27.88 | A693 |
| ATOM | 3031 | S21 | WAY | 169 | 69.757 | 38.213 | 21.577 | 1.00 | 24.43 | A693 |
| ATOM | 3032 | C16 | WAY | 169 | 71.513 | 38.570 | 21.438 | 1.00 | 29.69 | A693 |
| ATOM | 3033 | C21 | WAY | 169 | 72.032 | 39.163 | 20.269 | 1.00 | 19.32 | A693 |
| ATOM | 3034 | C20 | WAY | 169 | 73.400 | 39.453 | 20.169 | 1.00 | 11.82 | A693 |
| ATOM | 3035 | C19 | WAY | 169 | 74.267 | 39.156 | 21.241 | 1.00 | 19.50 | A693 |
| ATOM | 3036 | C18 | WAY | 169 | 73.748 | 38.564 | 22.402 | 1.00 | 11.88 | A693 |
| ATOM | 3037 | C17 | WAY | 169 | 72.382 | 38.272 | 22.507 | 1.00 | 26.57 | A693 |
| ATOM | 3038 | O33 | WAY | 169 | 75.623 | 39.445 | 21.141 | 1.00 | 16.99 | A693 |
| ATOM | 3039 | C36 | WAY | 169 | 76.504 | 39.509 | 22.271 | 1.00 | 12.69 | A693 |
| ATOM | 3040 | O15 | WAY | 169 | 69.030 | 39.032 | 20.657 | 1.00 | 13.98 | A693 |
| ATOM | 3041 | O14 | WAY | 169 | 69.419 | 38.338 | 22.942 | 1.00 | 22.94 | A693 |
| ATOM | 3042 | C7 | WAY | 169 | 70.780 | 36.256 | 18.621 | 1.00 | 30.48 | A693 |
| ATOM | 3043 | N9 | WAY | 169 | 71.192 | 36.946 | 17.553 | 1.00 | 10.00 | A693 |
| ATOM | 3044 | O10 | WAY | 169 | 72.581 | 37.127 | 17.426 | 1.00 | 38.25 | A693 |
| ATOM | 3045 | O8 | WAY | 169 | 71.614 | 35.847 | 19.414 | 1.00 | 39.46 | A693 |
| ATOM | 3046 | C29 | WAY | 169 | 66.584 | 36.175 | 21.566 | 1.00 | 46.13 | A693 |
| ATOM | 1505 | CB | THR | 7 | 40.443 | 57.305 | 5.225 | 1.00 | 21.20 | B_13 |
| ATOM | 1506 | OG1 | THR | 7 | 39.149 | 56.999 | 5.762 | 1.00 | 25.31 | B_13 |
| ATOM | 1508 | CG2 | THR | 7 | 41.017 | 56.087 | 4.541 | 1.00 | 23.15 | B_13 |
| ATOM | 1509 | C | THR | 7 | 40.920 | 59.113 | 6.901 | 1.00 | 32.45 | B_13 |
| ATOM | 1510 | O | THR | 7 | 41.453 | 59.582 | 7.908 | 1.00 | 36.97 | B_13 |
| ATOM | 1513 | N | THR | 7 | 41.386 | 56.786 | 7.488 | 1.00 | 34.12 | B_13 |
| ATOM | 1515 | CA | THR | 7 | 41.371 | 57.761 | 6.365 | 1.00 | 26.16 | B_13 |
| ATOM | 1516 | N | LEU | 8 | 39.907 | 59.694 | 6.265 | 1.00 | 23.60 | B_13 |
| ATOM | 1518 | CA | LEU | 8 | 39.387 | 60.984 | 6.649 | 1.00 | 22.66 | B_13 |
| ATOM | 1519 | CB | LEU | 8 | 38.113 | 60.848 | 7.503 | 1.00 | 21.78 | B_13 |
| ATOM | 1520 | CG | LEU | 8 | 36.860 | 61.484 | 6.863 | 1.00 | 27.13 | B_13 |
| ATOM | 1521 | CD1 | LEU | 8 | 36.996 | 63.016 | 6.705 | 1.00 | 19.05 | B_13 |
| ATOM | 1522 | CD2 | LEU | 8 | 36.622 | 60.854 | 5.510 | 1.00 | 19.23 | B_13 |
| ATOM | 1523 | C | LEU | 8 | 40.432 | 61.896 | 7.298 | 1.00 | 27.16 | B_13 |
| ATOM | 1524 | O | LEU | 8 | 41.077 | 62.667 | 6.597 | 1.00 | 46.24 | B_13 |
| ATOM | 1525 | N | LYS | 9 | 40.615 | 61.804 | 8.618 | 1.00 | 27.84 | B_13 |
| ATOM | 1527 | CA | LYS | 9 | 41.572 | 62.674 | 9.306 | 1.00 | 15.20 | B_13 |
| ATOM | 1528 | CB | LYS | 9 | 41.147 | 64.143 | 9.148 | 1.00 | 32.32 | B_13 |
| ATOM | 1529 | CG | LYS | 9 | 39.663 | 64.342 | 8.853 | 1.00 | 29.47 | B_13 |
| ATOM | 1530 | CD | LYS | 9 | 38.788 | 64.243 | 10.084 | 1.00 | 28.34 | B_13 |

54/75

| | | | | | | | | | | |
|------|------|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 1531 | CE | LYS | 9 | 38.830 | 65.556 | 10.842 | 1.00 | 18.48 | B_13 |
| ATOM | 1532 | NZ | LYS | 9 | 38.732 | 66.725 | 9.888 | 1.00 | 33.19 | B_13 |
| ATOM | 1536 | C | LYS | 9 | 41.809 | 62.384 | 10.780 | 1.00 | 20.69 | B_13 |
| ATOM | 1537 | O | LYS | 9 | 41.268 | 61.428 | 11.334 | 1.00 | 25.62 | B_13 |
| ATOM | 1538 | N | TRP | 10 | 42.654 | 63.208 | 11.390 | 1.00 | 12.09 | B_13 |
| ATOM | 1540 | CA | TRP | 10 | 42.988 | 63.112 | 12.813 | 1.00 | 21.78 | B_13 |
| ATOM | 1541 | CB | TRP | 10 | 44.403 | 63.660 | 13.048 | 1.00 | 23.03 | B_13 |
| ATOM | 1542 | CG | TRP | 10 | 45.499 | 62.890 | 12.349 | 1.00 | 27.60 | B_13 |
| ATOM | 1543 | CD2 | TRP | 10 | 46.077 | 61.650 | 12.762 | 1.00 | 27.28 | B_13 |
| ATOM | 1544 | CE2 | TRP | 10 | 47.071 | 61.302 | 11.829 | 1.00 | 22.11 | B_13 |
| ATOM | 1545 | CE3 | TRP | 10 | 45.859 | 60.781 | 13.847 | 1.00 | 11.66 | B_13 |
| ATOM | 1546 | CD1 | TRP | 10 | 46.153 | 63.247 | 11.198 | 1.00 | 21.84 | B_13 |
| ATOM | 1547 | NE1 | TRP | 10 | 47.094 | 62.305 | 10.873 | 1.00 | 10.00 | B_13 |
| ATOM | 1549 | CZ2 | TRP | 10 | 47.847 | 60.143 | 11.929 | 1.00 | 25.24 | B_13 |
| ATOM | 1550 | CZ3 | TRP | 10 | 46.632 | 59.622 | 13.951 | 1.00 | 22.71 | B_13 |
| ATOM | 1551 | CH2 | TRP | 10 | 47.611 | 59.317 | 12.999 | 1.00 | 15.23 | B_13 |
| ATOM | 1552 | C | TRP | 10 | 41.987 | 63.915 | 13.679 | 1.00 | 30.88 | B_13 |
| ATOM | 1553 | O | TRP | 10 | 41.673 | 65.062 | 13.359 | 1.00 | 32.03 | B_13 |
| ATOM | 1554 | N | SER | 11 | 41.495 | 63.316 | 14.765 | 1.00 | 35.64 | B_13 |
| ATOM | 1556 | CA | SER | 11 | 40.548 | 63.981 | 15.665 | 1.00 | 30.37 | B_13 |
| ATOM | 1557 | CB | SER | 11 | 39.498 | 62.995 | 16.176 | 1.00 | 31.03 | B_13 |
| ATOM | 1558 | OG | SER | 11 | 38.485 | 62.815 | 15.202 | 1.00 | 41.11 | B_13 |
| ATOM | 1560 | C | SER | 11 | 41.206 | 64.691 | 16.840 | 1.00 | 20.70 | B_13 |
| ATOM | 1561 | O | SER | 11 | 40.558 | 65.002 | 17.838 | 1.00 | 36.52 | B_13 |
| ATOM | 1562 | N | LYS | 12 | 42.504 | 64.910 | 16.731 | 1.00 | 23.56 | B_13 |
| ATOM | 1564 | CA | LYS | 12 | 43.257 | 65.607 | 17.756 | 1.00 | 15.00 | B_13 |
| ATOM | 1565 | CB | LYS | 12 | 43.991 | 64.631 | 18.688 | 1.00 | 18.58 | B_13 |
| ATOM | 1566 | CG | LYS | 12 | 44.658 | 63.452 | 18.010 | 1.00 | 15.94 | B_13 |
| ATOM | 1567 | CD | LYS | 12 | 45.456 | 62.589 | 19.007 | 1.00 | 23.03 | B_13 |
| ATOM | 1568 | CE | LYS | 12 | 44.593 | 61.715 | 19.933 | 1.00 | 27.10 | B_13 |
| ATOM | 1569 | NZ | LYS | 12 | 44.075 | 62.402 | 21.157 | 1.00 | 34.75 | B_13 |
| ATOM | 1573 | C | LYS | 12 | 44.200 | 66.453 | 16.914 | 1.00 | 25.03 | B_13 |
| ATOM | 1574 | O | LYS | 12 | 44.567 | 66.039 | 15.808 | 1.00 | 25.20 | B_13 |
| ATOM | 1575 | N | MET | 13 | 44.536 | 67.647 | 17.401 | 1.00 | 18.44 | B_13 |
| ATOM | 1577 | CA | MET | 13 | 45.377 | 68.582 | 16.663 | 1.00 | 24.63 | B_13 |
| ATOM | 1578 | CB | MET | 13 | 44.864 | 70.015 | 16.880 | 1.00 | 13.15 | B_13 |
| ATOM | 1579 | CG | MET | 13 | 43.421 | 70.253 | 16.419 | 1.00 | 21.56 | B_13 |
| ATOM | 1580 | SD | MET | 13 | 43.167 | 70.131 | 14.616 | 1.00 | 31.39 | B_13 |
| ATOM | 1581 | CE | MET | 13 | 41.433 | 69.678 | 14.474 | 1.00 | 24.70 | B_13 |
| ATOM | 1582 | C | MET | 13 | 46.850 | 68.468 | 17.034 | 1.00 | 11.65 | B_13 |
| ATOM | 1583 | O | MET | 13 | 47.728 | 68.815 | 16.247 | 1.00 | 14.33 | B_13 |
| ATOM | 1584 | N | ASN | 14 | 47.103 | 67.985 | 18.242 | 1.00 | 16.99 | B_13 |
| ATOM | 1586 | CA | ASN | 14 | 48.448 | 67.793 | 18.760 | 1.00 | 24.42 | B_13 |
| ATOM | 1587 | CB | ASN | 14 | 48.437 | 68.006 | 20.268 | 1.00 | 17.84 | B_13 |
| ATOM | 1588 | CG | ASN | 14 | 47.896 | 69.356 | 20.633 | 1.00 | 35.10 | B_13 |
| ATOM | 1589 | OD1 | ASN | 14 | 48.614 | 70.346 | 20.560 | 1.00 | 34.88 | B_13 |
| ATOM | 1590 | ND2 | ASN | 14 | 46.610 | 69.424 | 20.955 | 1.00 | 32.98 | B_13 |
| ATOM | 1593 | C | ASN | 14 | 48.831 | 66.364 | 18.421 | 1.00 | 22.70 | B_13 |
| ATOM | 1594 | O | ASN | 14 | 48.278 | 65.405 | 18.976 | 1.00 | 26.03 | B_13 |
| ATOM | 1595 | N | LEU | 15 | 49.706 | 66.228 | 17.432 | 1.00 | 18.07 | B_13 |
| ATOM | 1597 | CA | LEU | 15 | 50.144 | 64.912 | 16.969 | 1.00 | 29.36 | B_13 |
| ATOM | 1598 | CB | LEU | 15 | 49.878 | 64.775 | 15.466 | 1.00 | 24.35 | B_13 |
| ATOM | 1599 | CG | LEU | 15 | 48.380 | 64.762 | 15.162 | 1.00 | 19.51 | B_13 |
| ATOM | 1600 | CD1 | LEU | 15 | 48.079 | 65.469 | 13.852 | 1.00 | 27.59 | B_13 |
| ATOM | 1601 | CD2 | LEU | 15 | 47.902 | 63.326 | 15.163 | 1.00 | 19.66 | B_13 |
| ATOM | 1602 | C | LEU | 15 | 51.613 | 64.704 | 17.257 | 1.00 | 28.48 | B_13 |
| ATOM | 1603 | O | LEU | 15 | 52.341 | 65.657 | 17.552 | 1.00 | 22.28 | B_13 |
| ATOM | 1604 | N | THR | 16 | 52.044 | 63.453 | 17.198 | 1.00 | 12.77 | B_13 |
| ATOM | 1606 | CA | THR | 16 | 53.433 | 63.158 | 17.446 | 1.00 | 16.59 | B_13 |
| ATOM | 1607 | CB | THR | 16 | 53.607 | 62.243 | 18.682 | 1.00 | 24.73 | B_13 |
| ATOM | 1608 | OG1 | THR | 16 | 52.912 | 61.005 | 18.481 | 1.00 | 12.79 | B_13 |
| ATOM | 1610 | CG2 | THR | 16 | 53.059 | 62.933 | 19.924 | 1.00 | 25.34 | B_13 |
| ATOM | 1611 | C | THR | 16 | 54.038 | 62.515 | 16.214 | 1.00 | 21.94 | B_13 |
| ATOM | 1612 | O | THR | 16 | 53.315 | 62.116 | 15.297 | 1.00 | 19.60 | B_13 |
| ATOM | 1613 | N | TYR | 17 | 55.365 | 62.453 | 16.184 | 1.00 | 18.25 | B_13 |
| ATOM | 1615 | CA | TYR | 17 | 56.092 | 61.810 | 15.097 | 1.00 | 19.54 | B_13 |
| ATOM | 1616 | CB | TYR | 17 | 56.300 | 62.753 | 13.910 | 1.00 | 16.87 | B_13 |
| ATOM | 1617 | CG | TYR | 17 | 57.277 | 63.892 | 14.116 | 1.00 | 27.90 | B_13 |
| ATOM | 1618 | CD1 | TYR | 17 | 56.839 | 65.135 | 14.587 | 1.00 | 13.93 | B_13 |
| ATOM | 1619 | CE1 | TYR | 17 | 57.700 | 66.221 | 14.652 | 1.00 | 17.08 | B_13 |
| ATOM | 1620 | CD2 | TYR | 17 | 58.613 | 63.764 | 13.723 | 1.00 | 14.99 | B_13 |
| ATOM | 1621 | CE2 | TYR | 17 | 59.479 | 64.841 | 13.777 | 1.00 | 25.98 | B_13 |
| ATOM | 1622 | CZ | TYR | 17 | 59.017 | 66.075 | 14.242 | 1.00 | 33.12 | B_13 |
| ATOM | 1623 | OH | TYR | 17 | 59.866 | 67.163 | 14.276 | 1.00 | 23.31 | B_13 |
| ATOM | 1625 | C | TYR | 17 | 57.417 | 61.318 | 15.650 | 1.00 | 18.57 | B_13 |
| ATOM | 1626 | O | TYR | 17 | 57.895 | 61.827 | 16.668 | 1.00 | 26.60 | B_13 |
| ATOM | 1627 | N | ARG | 18 | 57.973 | 60.286 | 15.030 | 1.00 | 13.01 | B_13 |

55/75

| | | | | | | | | | | |
|------|------|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 1629 | CA | ARG | 18 | 59.245 | 59.750 | 15.492 | 1.00 | 18.74 | B_13 |
| ATOM | 1630 | CB | ARG | 18 | 59.033 | 58.589 | 16.473 | 1.00 | 11.96 | B_13 |
| ATOM | 1631 | CG | ARG | 18 | 60.320 | 57.911 | 16.970 | 1.00 | 15.06 | B_13 |
| ATOM | 1632 | CD | ARG | 18 | 60.012 | 56.596 | 17.690 | 1.00 | 11.72 | B_13 |
| ATOM | 1633 | NE | ARG | 18 | 61.165 | 55.689 | 17.752 | 1.00 | 10.00 | B_13 |
| ATOM | 1635 | CZ | ARG | 18 | 61.134 | 54.428 | 18.181 | 1.00 | 24.87 | B_13 |
| ATOM | 1636 | NH1 | ARG | 18 | 60.004 | 53.882 | 18.614 | 1.00 | 13.34 | B_13 |
| ATOM | 1639 | NH2 | ARG | 18 | 62.247 | 53.703 | 18.169 | 1.00 | 20.03 | B_13 |
| ATOM | 1642 | C | ARG | 18 | 60.076 | 59.309 | 14.307 | 1.00 | 13.14 | B_13 |
| ATOM | 1643 | O | ARG | 18 | 59.598 | 58.588 | 13.434 | 1.00 | 14.10 | B_13 |
| ATOM | 1644 | N | ILE | 19 | 61.304 | 59.813 | 14.252 | 1.00 | 15.55 | B_13 |
| ATOM | 1646 | CA | ILE | 19 | 62.238 | 59.476 | 13.193 | 1.00 | 10.41 | B_13 |
| ATOM | 1647 | CB | ILE | 19 | 63.307 | 60.603 | 13.054 | 1.00 | 17.20 | B_13 |
| ATOM | 1648 | CG2 | ILE | 19 | 64.273 | 60.307 | 11.903 | 1.00 | 16.57 | B_13 |
| ATOM | 1649 | CG1 | ILE | 19 | 62.613 | 61.952 | 12.836 | 1.00 | 15.47 | B_13 |
| ATOM | 1650 | CD1 | ILE | 19 | 63.543 | 63.110 | 12.783 | 1.00 | 14.99 | B_13 |
| ATOM | 1651 | C | ILE | 19 | 62.870 | 58.166 | 13.673 | 1.00 | 10.00 | B_13 |
| ATOM | 1652 | O | ILE | 19 | 63.829 | 58.179 | 14.434 | 1.00 | 10.00 | B_13 |
| ATOM | 1653 | N | VAL | 20 | 62.289 | 57.037 | 13.276 | 1.00 | 17.84 | B_13 |
| ATOM | 1655 | CA | VAL | 20 | 62.785 | 55.716 | 13.696 | 1.00 | 16.43 | B_13 |
| ATOM | 1656 | CB | VAL | 20 | 61.911 | 54.570 | 13.138 | 1.00 | 13.17 | B_13 |
| ATOM | 1657 | CG1 | VAL | 20 | 62.519 | 53.208 | 13.493 | 1.00 | 10.00 | B_13 |
| ATOM | 1658 | CG2 | VAL | 20 | 60.521 | 54.673 | 13.698 | 1.00 | 10.00 | B_13 |
| ATOM | 1659 | C | VAL | 20 | 64.268 | 55.449 | 13.387 | 1.00 | 16.02 | B_13 |
| ATOM | 1660 | O | VAL | 20 | 65.001 | 54.909 | 14.218 | 1.00 | 21.07 | B_13 |
| ATOM | 1661 | N | ASN | 21 | 64.698 | 55.762 | 12.177 | 1.00 | 10.00 | B_13 |
| ATOM | 1663 | CA | ASN | 21 | 66.098 | 55.571 | 11.830 | 1.00 | 22.13 | B_13 |
| ATOM | 1664 | CB | ASN | 21 | 66.392 | 54.128 | 11.386 | 1.00 | 19.75 | B_13 |
| ATOM | 1665 | CG | ASN | 21 | 65.549 | 53.673 | 10.212 | 1.00 | 17.63 | B_13 |
| ATOM | 1666 | OD1 | ASN | 21 | 65.329 | 52.477 | 10.042 | 1.00 | 31.82 | B_13 |
| ATOM | 1667 | ND2 | ASN | 21 | 65.109 | 54.602 | 9.375 | 1.00 | 11.42 | B_13 |
| ATOM | 1670 | C | ASN | 21 | 66.504 | 56.645 | 10.821 | 1.00 | 10.14 | B_13 |
| ATOM | 1671 | O | ASN | 21 | 65.639 | 57.377 | 10.340 | 1.00 | 11.74 | B_13 |
| ATOM | 1672 | N | TYR | 22 | 67.787 | 56.759 | 10.498 | 1.00 | 12.25 | B_13 |
| ATOM | 1674 | CA | TYR | 22 | 68.233 | 57.829 | 9.602 | 1.00 | 12.46 | B_13 |
| ATOM | 1675 | CB | TYR | 22 | 69.136 | 58.800 | 10.383 | 1.00 | 23.15 | B_13 |
| ATOM | 1676 | CG | TYR | 22 | 68.461 | 59.584 | 11.492 | 1.00 | 21.95 | B_13 |
| ATOM | 1677 | CD1 | TYR | 22 | 68.221 | 60.945 | 11.348 | 1.00 | 22.29 | B_13 |
| ATOM | 1678 | CE1 | TYR | 22 | 67.625 | 61.678 | 12.347 | 1.00 | 10.00 | B_13 |
| ATOM | 1679 | CD2 | TYR | 22 | 68.077 | 58.974 | 12.687 | 1.00 | 13.42 | B_13 |
| ATOM | 1680 | CE2 | TYR | 22 | 67.471 | 59.710 | 13.693 | 1.00 | 14.69 | B_13 |
| ATOM | 1681 | CZ | TYR | 22 | 67.254 | 61.064 | 13.505 | 1.00 | 12.89 | B_13 |
| ATOM | 1682 | OH | TYR | 22 | 66.660 | 61.829 | 14.466 | 1.00 | 16.56 | B_13 |
| ATOM | 1684 | C | TYR | 22 | 68.988 | 57.395 | 8.359 | 1.00 | 11.62 | B_13 |
| ATOM | 1685 | O | TYR | 22 | 69.793 | 56.478 | 8.407 | 1.00 | 16.23 | B_13 |
| ATOM | 1686 | N | THR | 23 | 68.792 | 58.111 | 7.261 | 1.00 | 10.39 | B_13 |
| ATOM | 1688 | CA | THR | 23 | 69.503 | 57.800 | 6.024 | 1.00 | 20.36 | B_13 |
| ATOM | 1689 | CB | THR | 23 | 68.909 | 58.582 | 4.829 | 1.00 | 16.21 | B_13 |
| ATOM | 1690 | OG1 | THR | 23 | 69.801 | 58.512 | 3.706 | 1.00 | 19.72 | B_13 |
| ATOM | 1692 | CG2 | THR | 23 | 68.663 | 60.039 | 5.206 | 1.00 | 16.62 | B_13 |
| ATOM | 1693 | C | THR | 23 | 70.990 | 58.153 | 6.163 | 1.00 | 17.35 | B_13 |
| ATOM | 1694 | O | THR | 23 | 71.377 | 58.958 | 7.024 | 1.00 | 13.88 | B_13 |
| ATOM | 1695 | N | PRO | 24 | 71.852 | 57.503 | 5.364 | 1.00 | 15.86 | B_13 |
| ATOM | 1696 | CD | PRO | 24 | 71.625 | 56.247 | 4.629 | 1.00 | 17.29 | B_13 |
| ATOM | 1697 | CA | PRO | 24 | 73.287 | 57.796 | 5.436 | 1.00 | 15.96 | B_13 |
| ATOM | 1698 | CB | PRO | 24 | 73.920 | 56.570 | 4.763 | 1.00 | 10.00 | B_13 |
| ATOM | 1699 | CG | PRO | 24 | 72.891 | 55.504 | 4.905 | 1.00 | 15.15 | B_13 |
| ATOM | 1700 | C | PRO | 24 | 73.635 | 59.069 | 4.668 | 1.00 | 27.08 | B_13 |
| ATOM | 1701 | O | PRO | 24 | 74.698 | 59.656 | 4.869 | 1.00 | 19.47 | B_13 |
| ATOM | 1702 | N | ASP | 25 | 72.728 | 59.489 | 3.794 | 1.00 | 16.99 | B_13 |
| ATOM | 1704 | CA | ASP | 25 | 72.927 | 60.663 | 2.958 | 1.00 | 10.00 | B_13 |
| ATOM | 1705 | CB | ASP | 25 | 71.792 | 60.758 | 1.953 | 1.00 | 11.53 | B_13 |
| ATOM | 1706 | CG | ASP | 25 | 71.665 | 59.521 | 1.105 | 1.00 | 33.88 | B_13 |
| ATOM | 1707 | OD1 | ASP | 25 | 70.570 | 59.311 | 0.556 | 1.00 | 22.66 | B_13 |
| ATOM | 1708 | OD2 | ASP | 25 | 72.653 | 58.762 | 0.980 | 1.00 | 29.59 | B_13 |
| ATOM | 1709 | C | ASP | 25 | 73.068 | 62.011 | 3.642 | 1.00 | 23.36 | B_13 |
| ATOM | 1710 | O | ASP | 25 | 73.694 | 62.916 | 3.093 | 1.00 | 20.32 | B_13 |
| ATOM | 1711 | N | MET | 26 | 72.480 | 62.158 | 4.826 | 1.00 | 18.44 | B_13 |
| ATOM | 1713 | CA | MET | 26 | 72.510 | 63.432 | 5.537 | 1.00 | 13.83 | B_13 |
| ATOM | 1714 | CB | MET | 26 | 71.154 | 64.151 | 5.368 | 1.00 | 10.00 | B_13 |
| ATOM | 1715 | CG | MET | 26 | 70.782 | 64.491 | 3.913 | 1.00 | 28.32 | B_13 |
| ATOM | 1716 | SD | MET | 26 | 69.016 | 64.786 | 3.599 | 1.00 | 12.18 | B_13 |
| ATOM | 1717 | CE | MET | 26 | 68.395 | 63.255 | 3.887 | 1.00 | 37.25 | B_13 |
| ATOM | 1718 | C | MET | 26 | 72.827 | 63.238 | 7.024 | 1.00 | 28.80 | B_13 |
| ATOM | 1719 | O | MET | 26 | 72.839 | 62.107 | 7.533 | 1.00 | 20.90 | B_13 |
| ATOM | 1720 | N | THR | 27 | 73.157 | 64.333 | 7.696 | 1.00 | 11.47 | B_13 |
| ATOM | 1722 | CA | THR | 27 | 73.456 | 64.292 | 9.121 | 1.00 | 13.94 | B_13 |

56/75

| | | | | | | | | | | |
|------|------|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 1723 | CB | THR | 27 | 74.117 | 65.605 | 9.602 | 1.00 | 33.46 | B_13 |
| ATOM | 1724 | OG1 | THR | 27 | 73.209 | 66.702 | 9.415 | 1.00 | 10.00 | B_13 |
| ATOM | 1726 | CG2 | THR | 27 | 75.405 | 65.863 | 8.818 | 1.00 | 16.30 | B_13 |
| ATOM | 1727 | C | THR | 27 | 72.135 | 64.113 | 9.861 | 1.00 | 10.67 | B_13 |
| ATOM | 1728 | O | THR | 27 | 71.072 | 64.343 | 9.281 | 1.00 | 16.26 | B_13 |
| ATOM | 1729 | N | HIS | 28 | 72.193 | 63.691 | 11.124 | 1.00 | 18.13 | B_13 |
| ATOM | 1731 | CA | HIS | 28 | 70.986 | 63.514 | 11.915 | 1.00 | 10.00 | B_13 |
| ATOM | 1732 | CB | HIS | 28 | 71.322 | 63.033 | 13.333 | 1.00 | 10.00 | B_13 |
| ATOM | 1733 | CG | HIS | 28 | 71.793 | 61.608 | 13.401 | 1.00 | 22.65 | B_13 |
| ATOM | 1734 | CD2 | HIS | 28 | 72.893 | 61.003 | 12.889 | 1.00 | 22.73 | B_13 |
| ATOM | 1735 | ND1 | HIS | 28 | 71.103 | 60.627 | 14.080 | 1.00 | 19.90 | B_13 |
| ATOM | 1737 | CE1 | HIS | 28 | 71.755 | 59.481 | 13.985 | 1.00 | 16.52 | B_13 |
| ATOM | 1738 | NE2 | HIS | 28 | 72.843 | 59.681 | 13.268 | 1.00 | 20.38 | B_13 |
| ATOM | 1740 | C | HIS | 28 | 70.281 | 64.870 | 11.957 | 1.00 | 29.38 | B_13 |
| ATOM | 1741 | O | HIS | 28 | 69.074 | 64.941 | 11.742 | 1.00 | 17.20 | B_13 |
| ATOM | 1742 | N | SER | 29 | 71.056 | 65.944 | 12.153 | 1.00 | 23.96 | B_13 |
| ATOM | 1744 | CA | SER | 29 | 70.533 | 67.322 | 12.192 | 1.00 | 15.01 | B_13 |
| ATOM | 1745 | CB | SER | 29 | 71.661 | 68.334 | 12.438 | 1.00 | 14.05 | B_13 |
| ATOM | 1746 | OG | SER | 29 | 72.117 | 68.303 | 13.770 | 1.00 | 18.32 | B_13 |
| ATOM | 1748 | C | SER | 29 | 69.808 | 67.729 | 10.909 | 1.00 | 10.95 | B_13 |
| ATOM | 1749 | O | SER | 29 | 68.732 | 68.314 | 10.971 | 1.00 | 24.24 | B_13 |
| ATOM | 1750 | N | GLU | 30 | 70.415 | 67.449 | 9.757 | 1.00 | 10.96 | B_13 |
| ATOM | 1752 | CA | GLU | 30 | 69.820 | 67.786 | 8.470 | 1.00 | 10.00 | B_13 |
| ATOM | 1753 | CB | GLU | 30 | 70.715 | 67.330 | 7.309 | 1.00 | 10.12 | B_13 |
| ATOM | 1754 | CG | GLU | 30 | 71.967 | 68.143 | 7.042 | 1.00 | 22.31 | B_13 |
| ATOM | 1755 | CD | GLU | 30 | 72.823 | 67.529 | 5.930 | 1.00 | 10.15 | B_13 |
| ATOM | 1756 | OE1 | GLU | 30 | 72.533 | 67.753 | 4.749 | 1.00 | 31.98 | B_13 |
| ATOM | 1757 | OE2 | GLU | 30 | 73.796 | 66.817 | 6.223 | 1.00 | 29.59 | B_13 |
| ATOM | 1758 | C | GLU | 30 | 68.481 | 67.073 | 8.336 | 1.00 | 20.17 | B_13 |
| ATOM | 1759 | O | GLU | 30 | 67.493 | 67.685 | 7.943 | 1.00 | 14.31 | B_13 |
| ATOM | 1760 | N | VAL | 31 | 68.451 | 65.777 | 8.665 | 1.00 | 19.26 | B_13 |
| ATOM | 1762 | CA | VAL | 31 | 67.228 | 64.989 | 8.536 | 1.00 | 14.22 | B_13 |
| ATOM | 1763 | CB | VAL | 31 | 67.472 | 63.487 | 8.716 | 1.00 | 17.05 | B_13 |
| ATOM | 1764 | CG1 | VAL | 31 | 66.144 | 62.749 | 8.791 | 1.00 | 28.55 | B_13 |
| ATOM | 1765 | CG2 | VAL | 31 | 68.269 | 62.935 | 7.548 | 1.00 | 10.54 | B_13 |
| ATOM | 1766 | C | VAL | 31 | 66.138 | 65.458 | 9.477 | 1.00 | 12.36 | B_13 |
| ATOM | 1767 | O | VAL | 31 | 64.963 | 65.488 | 9.093 | 1.00 | 12.83 | B_13 |
| ATOM | 1768 | N | GLU | 32 | 66.530 | 65.805 | 10.703 | 1.00 | 20.46 | B_13 |
| ATOM | 1770 | CA | GLU | 32 | 65.596 | 66.306 | 11.710 | 1.00 | 16.04 | B_13 |
| ATOM | 1771 | CB | GLU | 32 | 66.269 | 66.365 | 13.094 | 1.00 | 14.71 | B_13 |
| ATOM | 1772 | CG | GLU | 32 | 66.512 | 64.985 | 13.741 | 1.00 | 23.30 | B_13 |
| ATOM | 1773 | CD | GLU | 32 | 67.724 | 64.930 | 14.700 | 1.00 | 21.41 | B_13 |
| ATOM | 1774 | OE1 | GLU | 32 | 68.229 | 63.823 | 15.003 | 1.00 | 15.79 | B_13 |
| ATOM | 1775 | OE2 | GLU | 32 | 68.183 | 65.985 | 15.157 | 1.00 | 13.71 | B_13 |
| ATOM | 1776 | C | GLU | 32 | 65.125 | 67.697 | 11.257 | 1.00 | 27.19 | B_13 |
| ATOM | 1777 | O | GLU | 32 | 63.951 | 68.042 | 11.383 | 1.00 | 19.82 | B_13 |
| ATOM | 1778 | N | LYS | 33 | 66.021 | 68.461 | 10.636 | 1.00 | 12.52 | B_13 |
| ATOM | 1780 | CA | LYS | 33 | 65.663 | 69.786 | 10.171 | 1.00 | 13.00 | B_13 |
| ATOM | 1781 | CB | LYS | 33 | 66.889 | 70.592 | 9.762 | 1.00 | 22.63 | B_13 |
| ATOM | 1782 | CG | LYS | 33 | 66.581 | 72.054 | 9.560 | 1.00 | 18.24 | B_13 |
| ATOM | 1783 | CD | LYS | 33 | 65.604 | 72.545 | 10.630 | 1.00 | 29.21 | B_13 |
| ATOM | 1784 | CE | LYS | 33 | 66.185 | 72.429 | 12.048 | 1.00 | 41.79 | B_13 |
| ATOM | 1785 | NZ | LYS | 33 | 65.181 | 71.939 | 13.054 | 1.00 | 20.17 | B_13 |
| ATOM | 1789 | C | LYS | 33 | 64.698 | 69.686 | 9.023 | 1.00 | 10.62 | B_13 |
| ATOM | 1790 | O | LYS | 33 | 63.734 | 70.437 | 8.971 | 1.00 | 22.94 | B_13 |
| ATOM | 1791 | N | ALA | 34 | 64.915 | 68.707 | 8.150 | 1.00 | 10.00 | B_13 |
| ATOM | 1793 | CA | ALA | 34 | 64.050 | 68.475 | 7.000 | 1.00 | 11.94 | B_13 |
| ATOM | 1794 | CB | ALA | 34 | 64.611 | 67.374 | 6.100 | 1.00 | 10.00 | B_13 |
| ATOM | 1795 | C | ALA | 34 | 62.640 | 68.115 | 7.423 | 1.00 | 10.00 | B_13 |
| ATOM | 1796 | O | ALA | 34 | 61.675 | 68.650 | 6.878 | 1.00 | 15.32 | B_13 |
| ATOM | 1797 | N | PHE | 35 | 62.510 | 67.208 | 8.387 | 1.00 | 21.32 | B_13 |
| ATOM | 1799 | CA | PHE | 35 | 61.187 | 66.789 | 8.852 | 1.00 | 18.32 | B_13 |
| ATOM | 1800 | CB | PHE | 35 | 61.267 | 65.451 | 9.614 | 1.00 | 25.48 | B_13 |
| ATOM | 1801 | CG | PHE | 35 | 61.620 | 64.260 | 8.735 | 1.00 | 14.33 | B_13 |
| ATOM | 1802 | CD1 | PHE | 35 | 61.149 | 64.171 | 7.427 | 1.00 | 17.91 | B_13 |
| ATOM | 1803 | CD2 | PHE | 35 | 62.436 | 63.240 | 9.217 | 1.00 | 18.05 | B_13 |
| ATOM | 1804 | CE1 | PHE | 35 | 61.486 | 63.086 | 6.610 | 1.00 | 18.49 | B_13 |
| ATOM | 1805 | CE2 | PHE | 35 | 62.778 | 62.158 | 8.413 | 1.00 | 15.01 | B_13 |
| ATOM | 1806 | CZ | PHE | 35 | 62.301 | 62.081 | 7.103 | 1.00 | 10.00 | B_13 |
| ATOM | 1807 | C | PHE | 35 | 60.428 | 67.862 | 9.658 | 1.00 | 18.68 | B_13 |
| ATOM | 1808 | O | PHE | 35 | 59.202 | 67.971 | 9.556 | 1.00 | 17.05 | B_13 |
| ATOM | 1809 | N | LYS | 36 | 61.160 | 68.664 | 10.425 | 1.00 | 16.30 | B_13 |
| ATOM | 1811 | CA | LYS | 36 | 60.579 | 69.749 | 11.229 | 1.00 | 19.34 | B_13 |
| ATOM | 1812 | CB | LYS | 36 | 61.676 | 70.420 | 12.052 | 1.00 | 24.61 | B_13 |
| ATOM | 1813 | CG | LYS | 36 | 61.200 | 71.293 | 13.191 | 1.00 | 18.38 | B_13 |
| ATOM | 1814 | CD | LYS | 36 | 62.408 | 71.795 | 13.962 | 1.00 | 19.34 | B_13 |
| ATOM | 1815 | CE | LYS | 36 | 62.067 | 72.267 | 15.356 | 1.00 | 21.80 | B_13 |

57/75

| | | | | | | | | | | |
|------|------|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 1816 | NZ | LYS | 36 | 63.299 | 72.615 | 16.118 | 1.00 | 27.76 | B_13 |
| ATOM | 1820 | C | LYS | 36 | 59.924 | 70.770 | 10.301 | 1.00 | 10.19 | B_13 |
| ATOM | 1821 | O | LYS | 36 | 58.788 | 71.183 | 10.528 | 1.00 | 14.95 | B_13 |
| ATOM | 1822 | N | LYS | 37 | 60.630 | 71.134 | 9.233 | 1.00 | 15.89 | B_13 |
| ATOM | 1824 | CA | LYS | 37 | 60.126 | 72.076 | 8.230 | 1.00 | 19.95 | B_13 |
| ATOM | 1825 | CB | LYS | 37 | 61.202 | 72.386 | 7.189 | 1.00 | 10.00 | B_13 |
| ATOM | 1826 | CG | LYS | 37 | 62.209 | 73.439 | 7.569 | 1.00 | 13.18 | B_13 |
| ATOM | 1827 | CD | LYS | 37 | 62.869 | 73.966 | 6.311 | 1.00 | 28.86 | B_13 |
| ATOM | 1828 | CE | LYS | 37 | 61.825 | 74.460 | 5.281 | 1.00 | 31.44 | B_13 |
| ATOM | 1829 | NZ | LYS | 37 | 60.878 | 75.512 | 5.772 | 1.00 | 26.23 | B_13 |
| ATOM | 1833 | C | LYS | 37 | 58.939 | 71.482 | 7.472 | 1.00 | 25.64 | B_13 |
| ATOM | 1834 | O | LYS | 37 | 57.968 | 72.177 | 7.161 | 1.00 | 24.39 | B_13 |
| ATOM | 1835 | N | ALA | 38 | 59.060 | 70.205 | 7.128 | 1.00 | 17.12 | B_13 |
| ATOM | 1837 | CA | ALA | 38 | 58.031 | 69.493 | 6.381 | 1.00 | 16.06 | B_13 |
| ATOM | 1838 | CB | ALA | 38 | 58.459 | 68.038 | 6.154 | 1.00 | 12.19 | B_13 |
| ATOM | 1839 | C | ALA | 38 | 56.692 | 69.557 | 7.094 | 1.00 | 11.12 | B_13 |
| ATOM | 1840 | O | ALA | 38 | 55.648 | 69.736 | 6.458 | 1.00 | 31.10 | B_13 |
| ATOM | 1841 | N | PHE | 39 | 56.732 | 69.393 | 8.417 | 1.00 | 21.01 | B_13 |
| ATOM | 1843 | CA | PHE | 39 | 55.540 | 69.446 | 9.257 | 1.00 | 10.85 | B_13 |
| ATOM | 1844 | CB | PHE | 39 | 55.841 | 68.833 | 10.639 | 1.00 | 14.45 | B_13 |
| ATOM | 1845 | CG | PHE | 39 | 55.851 | 67.325 | 10.659 | 1.00 | 21.88 | B_13 |
| ATOM | 1846 | CD1 | PHE | 39 | 57.016 | 66.625 | 10.954 | 1.00 | 16.88 | B_13 |
| ATOM | 1847 | CD2 | PHE | 39 | 54.675 | 66.599 | 10.442 | 1.00 | 22.14 | B_13 |
| ATOM | 1848 | CE1 | PHE | 39 | 57.010 | 65.223 | 11.037 | 1.00 | 17.95 | B_13 |
| ATOM | 1849 | CE2 | PHE | 39 | 54.655 | 65.190 | 10.522 | 1.00 | 17.22 | B_13 |
| ATOM | 1850 | CZ | PHE | 39 | 55.823 | 64.503 | 10.823 | 1.00 | 13.51 | B_13 |
| ATOM | 1851 | C | PHE | 39 | 55.044 | 70.898 | 9.426 | 1.00 | 19.98 | B_13 |
| ATOM | 1852 | O | PHE | 39 | 53.839 | 71.160 | 9.393 | 1.00 | 14.30 | B_13 |
| ATOM | 1853 | N | LYS | 40 | 55.981 | 71.826 | 9.611 | 1.00 | 20.03 | B_13 |
| ATOM | 1855 | CA | LYS | 40 | 55.681 | 73.245 | 9.795 | 1.00 | 18.64 | B_13 |
| ATOM | 1856 | CB | LYS | 40 | 56.989 | 74.011 | 10.020 | 1.00 | 19.28 | B_13 |
| ATOM | 1857 | CG | LYS | 40 | 57.064 | 75.392 | 9.440 | 1.00 | 26.34 | B_13 |
| ATOM | 1858 | CD | LYS | 40 | 58.288 | 76.093 | 9.974 | 1.00 | 18.46 | B_13 |
| ATOM | 1859 | CE | LYS | 40 | 58.021 | 76.673 | 11.339 | 1.00 | 20.86 | B_13 |
| ATOM | 1860 | NZ | LYS | 40 | 57.053 | 77.814 | 11.232 | 1.00 | 27.28 | B_13 |
| ATOM | 1864 | C | LYS | 40 | 54.899 | 73.790 | 8.612 | 1.00 | 20.57 | B_13 |
| ATOM | 1865 | O | LYS | 40 | 54.034 | 74.654 | 8.756 | 1.00 | 22.54 | B_13 |
| ATOM | 1866 | N | VAL | 41 | 55.216 | 73.251 | 7.445 | 1.00 | 17.15 | B_13 |
| ATOM | 1868 | CA | VAL | 41 | 54.565 | 73.576 | 6.184 | 1.00 | 19.19 | B_13 |
| ATOM | 1869 | CB | VAL | 41 | 55.095 | 72.566 | 5.086 | 1.00 | 17.28 | B_13 |
| ATOM | 1870 | CG1 | VAL | 41 | 53.987 | 72.064 | 4.160 | 1.00 | 10.00 | B_13 |
| ATOM | 1871 | CG2 | VAL | 41 | 56.224 | 73.191 | 4.293 | 1.00 | 19.38 | B_13 |
| ATOM | 1872 | C | VAL | 41 | 53.026 | 73.472 | 6.354 | 1.00 | 20.38 | B_13 |
| ATOM | 1873 | O | VAL | 41 | 52.268 | 74.280 | 5.810 | 1.00 | 28.57 | B_13 |
| ATOM | 1874 | N | TRP | 42 | 52.587 | 72.511 | 7.163 | 1.00 | 23.10 | B_13 |
| ATOM | 1876 | CA | TRP | 42 | 51.166 | 72.265 | 7.403 | 1.00 | 19.29 | B_13 |
| ATOM | 1877 | CB | TRP | 42 | 50.912 | 70.757 | 7.487 | 1.00 | 22.19 | B_13 |
| ATOM | 1878 | CG | TRP | 42 | 51.437 | 70.007 | 6.313 | 1.00 | 19.32 | B_13 |
| ATOM | 1879 | CD2 | TRP | 42 | 50.836 | 69.909 | 5.015 | 1.00 | 31.02 | B_13 |
| ATOM | 1880 | CE2 | TRP | 42 | 51.659 | 69.067 | 4.238 | 1.00 | 22.49 | B_13 |
| ATOM | 1881 | CE3 | TRP | 42 | 49.677 | 70.448 | 4.434 | 1.00 | 15.54 | B_13 |
| ATOM | 1882 | CD1 | TRP | 42 | 52.571 | 69.251 | 6.269 | 1.00 | 14.04 | B_13 |
| ATOM | 1883 | NE1 | TRP | 42 | 52.710 | 68.681 | 5.027 | 1.00 | 13.55 | B_13 |
| ATOM | 1885 | CZ2 | TRP | 42 | 51.360 | 68.752 | 2.912 | 1.00 | 18.87 | B_13 |
| ATOM | 1886 | CZ3 | TRP | 42 | 49.383 | 70.132 | 3.116 | 1.00 | 13.33 | B_13 |
| ATOM | 1887 | CH2 | TRP | 42 | 50.219 | 69.294 | 2.370 | 1.00 | 20.30 | B_13 |
| ATOM | 1888 | C | TRP | 42 | 50.617 | 72.926 | 8.660 | 1.00 | 24.68 | B_13 |
| ATOM | 1889 | O | TRP | 42 | 49.455 | 73.339 | 8.688 | 1.00 | 20.93 | B_13 |
| ATOM | 1890 | N | SER | 43 | 51.432 | 72.987 | 9.710 | 1.00 | 20.63 | B_13 |
| ATOM | 1892 | CA | SER | 43 | 51.007 | 73.601 | 10.968 | 1.00 | 22.47 | B_13 |
| ATOM | 1893 | CB | SER | 43 | 51.955 | 73.231 | 12.116 | 1.00 | 10.00 | B_13 |
| ATOM | 1894 | OG | SER | 43 | 53.265 | 73.716 | 11.891 | 1.00 | 33.50 | B_13 |
| ATOM | 1896 | C | SER | 43 | 50.913 | 75.122 | 10.829 | 1.00 | 14.99 | B_13 |
| ATOM | 1897 | O | SER | 43 | 50.224 | 75.784 | 11.595 | 1.00 | 11.58 | B_13 |
| ATOM | 1898 | N | ASP | 44 | 51.613 | 75.667 | 9.843 | 1.00 | 26.20 | B_13 |
| ATOM | 1900 | CA | ASP | 44 | 51.595 | 77.100 | 9.617 | 1.00 | 22.11 | B_13 |
| ATOM | 1901 | CB | ASP | 44 | 52.620 | 77.485 | 8.549 | 1.00 | 11.09 | B_13 |
| ATOM | 1902 | CG | ASP | 44 | 54.000 | 77.751 | 9.125 | 1.00 | 18.45 | B_13 |
| ATOM | 1903 | OD1 | ASP | 44 | 54.903 | 78.114 | 8.347 | 1.00 | 17.67 | B_13 |
| ATOM | 1904 | OD2 | ASP | 44 | 54.195 | 77.602 | 10.345 | 1.00 | 21.44 | B_13 |
| ATOM | 1905 | C | ASP | 44 | 50.216 | 77.575 | 9.190 | 1.00 | 32.83 | B_13 |
| ATOM | 1906 | O | ASP | 44 | 49.795 | 78.677 | 9.549 | 1.00 | 34.78 | B_13 |
| ATOM | 1907 | N | VAL | 45 | 49.508 | 76.735 | 8.439 | 1.00 | 31.40 | B_13 |
| ATOM | 1909 | CA | VAL | 45 | 48.191 | 77.094 | 7.932 | 1.00 | 14.00 | B_13 |
| ATOM | 1910 | CB | VAL | 45 | 48.121 | 76.872 | 6.401 | 1.00 | 15.73 | B_13 |
| ATOM | 1911 | CG1 | VAL | 45 | 49.123 | 77.755 | 5.707 | 1.00 | 19.37 | B_13 |
| ATOM | 1912 | CG2 | VAL | 45 | 48.407 | 75.409 | 6.055 | 1.00 | 10.00 | B_13 |

58/75

| | | | | | | | | | | |
|------|------|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 1913 | C | VAL | 45 | 47.054 | 76.333 | 8.575 | 1.00 | 18.43 | B_13 |
| ATOM | 1914 | O | VAL | 45 | 45.954 | 76.304 | 8.026 | 1.00 | 26.09 | B_13 |
| ATOM | 1915 | N | THR | 46 | 47.295 | 75.754 | 9.747 | 1.00 | 18.49 | B_13 |
| ATOM | 1917 | CA | THR | 46 | 46.262 | 74.963 | 10.408 | 1.00 | 21.92 | B_13 |
| ATOM | 1918 | CB | THR | 46 | 46.222 | 73.529 | 9.751 | 1.00 | 27.61 | B_13 |
| ATOM | 1919 | OG1 | THR | 46 | 44.876 | 73.047 | 9.661 | 1.00 | 28.78 | B_13 |
| ATOM | 1921 | CG2 | THR | 46 | 47.054 | 72.550 | 10.522 | 1.00 | 10.65 | B_13 |
| ATOM | 1922 | C | THR | 46 | 46.505 | 74.931 | 11.932 | 1.00 | 18.41 | B_13 |
| ATOM | 1923 | O | THR | 46 | 47.554 | 75.363 | 12.411 | 1.00 | 18.63 | B_13 |
| ATOM | 1924 | N | PRO | 47 | 45.519 | 74.467 | 12.717 | 1.00 | 16.81 | B_13 |
| ATOM | 1925 | CD | PRO | 47 | 44.113 | 74.209 | 12.348 | 1.00 | 32.80 | B_13 |
| ATOM | 1926 | CA | PRO | 47 | 45.691 | 74.407 | 14.169 | 1.00 | 13.66 | B_13 |
| ATOM | 1927 | CB | PRO | 47 | 44.256 | 74.489 | 14.675 | 1.00 | 30.52 | B_13 |
| ATOM | 1928 | CG | PRO | 47 | 43.519 | 73.692 | 13.638 | 1.00 | 29.25 | B_13 |
| ATOM | 1929 | C | PRO | 47 | 46.346 | 73.105 | 14.622 | 1.00 | 28.40 | B_13 |
| ATOM | 1930 | O | PRO | 47 | 46.037 | 72.597 | 15.705 | 1.00 | 29.19 | B_13 |
| ATOM | 1931 | N | LEU | 48 | 47.220 | 72.547 | 13.784 | 1.00 | 27.10 | B_13 |
| ATOM | 1933 | CA | LEU | 48 | 47.915 | 71.302 | 14.124 | 1.00 | 21.49 | B_13 |
| ATOM | 1934 | CB | LEU | 48 | 48.087 | 70.418 | 12.885 | 1.00 | 16.21 | B_13 |
| ATOM | 1935 | CG | LEU | 48 | 46.924 | 69.476 | 12.538 | 1.00 | 15.14 | B_13 |
| ATOM | 1936 | CD1 | LEU | 48 | 45.618 | 70.049 | 13.000 | 1.00 | 26.83 | B_13 |
| ATOM | 1937 | CD2 | LEU | 48 | 46.894 | 69.206 | 11.035 | 1.00 | 32.93 | B_13 |
| ATOM | 1938 | C | LEU | 48 | 49.262 | 71.611 | 14.771 | 1.00 | 16.35 | B_13 |
| ATOM | 1939 | O | LEU | 48 | 49.885 | 72.648 | 14.498 | 1.00 | 26.65 | B_13 |
| ATOM | 1940 | N | ASN | 49 | 49.691 | 70.744 | 15.669 | 1.00 | 18.84 | B_13 |
| ATOM | 1942 | CA | ASN | 49 | 50.956 | 70.940 | 16.354 | 1.00 | 25.67 | B_13 |
| ATOM | 1943 | CB | ASN | 49 | 50.741 | 71.205 | 17.846 | 1.00 | 23.64 | B_13 |
| ATOM | 1944 | CG | ASN | 49 | 49.734 | 72.301 | 18.100 | 1.00 | 23.64 | B_13 |
| ATOM | 1945 | OD1 | ASN | 49 | 48.895 | 72.192 | 18.989 | 1.00 | 33.47 | B_13 |
| ATOM | 1946 | ND2 | ASN | 49 | 49.796 | 73.359 | 17.305 | 1.00 | 37.40 | B_13 |
| ATOM | 1949 | C | ASN | 49 | 51.695 | 69.643 | 16.195 | 1.00 | 22.08 | B_13 |
| ATOM | 1950 | O | ASN | 49 | 51.087 | 68.577 | 16.252 | 1.00 | 23.48 | B_13 |
| ATOM | 1951 | N | PHE | 50 | 52.994 | 69.723 | 15.951 | 1.00 | 25.59 | B_13 |
| ATOM | 1953 | CA | PHE | 50 | 53.762 | 68.510 | 15.806 | 1.00 | 19.57 | B_13 |
| ATOM | 1954 | CB | PHE | 50 | 54.258 | 68.343 | 14.380 | 1.00 | 12.47 | B_13 |
| ATOM | 1955 | CG | PHE | 50 | 53.161 | 68.024 | 13.432 | 1.00 | 14.47 | B_13 |
| ATOM | 1956 | CD1 | PHE | 50 | 52.665 | 68.989 | 12.581 | 1.00 | 17.81 | B_13 |
| ATOM | 1957 | CD2 | PHE | 50 | 52.566 | 66.770 | 13.445 | 1.00 | 14.44 | B_13 |
| ATOM | 1958 | CE1 | PHE | 50 | 51.585 | 68.705 | 11.754 | 1.00 | 23.43 | B_13 |
| ATOM | 1959 | CE2 | PHE | 50 | 51.488 | 66.482 | 12.624 | 1.00 | 20.62 | B_13 |
| ATOM | 1960 | CZ | PHE | 50 | 50.999 | 67.447 | 11.781 | 1.00 | 13.34 | B_13 |
| ATOM | 1961 | C | PHE | 50 | 54.858 | 68.419 | 16.826 | 1.00 | 23.56 | B_13 |
| ATOM | 1962 | O | PHE | 50 | 55.720 | 69.299 | 16.922 | 1.00 | 20.28 | B_13 |
| ATOM | 1963 | N | THR | 51 | 54.728 | 67.387 | 17.651 | 1.00 | 26.45 | B_13 |
| ATOM | 1965 | CA | THR | 51 | 55.650 | 67.090 | 18.725 | 1.00 | 29.37 | B_13 |
| ATOM | 1966 | CB | THR | 51 | 54.851 | 66.834 | 20.024 | 1.00 | 28.17 | B_13 |
| ATOM | 1967 | OG1 | THR | 51 | 53.946 | 65.738 | 19.824 | 1.00 | 40.86 | B_13 |
| ATOM | 1969 | CG2 | THR | 51 | 54.032 | 68.078 | 20.393 | 1.00 | 25.37 | B_13 |
| ATOM | 1970 | C | THR | 51 | 56.435 | 65.838 | 18.331 | 1.00 | 21.26 | B_13 |
| ATOM | 1971 | O | THR | 51 | 55.849 | 64.849 | 17.882 | 1.00 | 17.45 | B_13 |
| ATOM | 1972 | N | ARG | 52 | 57.755 | 65.889 | 18.477 | 1.00 | 15.17 | B_13 |
| ATOM | 1974 | CA | ARG | 52 | 58.604 | 64.752 | 18.126 | 1.00 | 20.79 | B_13 |
| ATOM | 1975 | CB | ARG | 52 | 59.868 | 65.241 | 17.429 | 1.00 | 20.81 | B_13 |
| ATOM | 1976 | CG | ARG | 52 | 60.871 | 64.160 | 17.110 | 1.00 | 19.06 | B_13 |
| ATOM | 1977 | CD | ARG | 52 | 62.208 | 64.808 | 16.880 | 1.00 | 22.17 | B_13 |
| ATOM | 1978 | NE | ARG | 52 | 63.293 | 63.848 | 16.904 | 1.00 | 18.57 | B_13 |
| ATOM | 1980 | CZ | ARG | 52 | 64.563 | 64.160 | 17.108 | 1.00 | 10.00 | B_13 |
| ATOM | 1981 | NH1 | ARG | 52 | 64.915 | 65.414 | 17.315 | 1.00 | 19.35 | B_13 |
| ATOM | 1984 | NH2 | ARG | 52 | 65.488 | 63.214 | 17.039 | 1.00 | 35.90 | B_13 |
| ATOM | 1987 | C | ARG | 52 | 58.995 | 63.903 | 19.328 | 1.00 | 22.29 | B_13 |
| ATOM | 1988 | O | ARG | 52 | 59.326 | 64.433 | 20.387 | 1.00 | 24.98 | B_13 |
| ATOM | 1989 | N | LEU | 53 | 59.013 | 62.586 | 19.140 | 1.00 | 19.90 | B_13 |
| ATOM | 1991 | CA | LEU | 53 | 59.378 | 61.660 | 20.203 | 1.00 | 27.02 | B_13 |
| ATOM | 1992 | CB | LEU | 53 | 58.279 | 60.625 | 20.434 | 1.00 | 16.80 | B_13 |
| ATOM | 1993 | CG | LEU | 53 | 56.859 | 61.138 | 20.639 | 1.00 | 23.45 | B_13 |
| ATOM | 1994 | CD1 | LEU | 53 | 55.943 | 59.943 | 20.884 | 1.00 | 24.07 | B_13 |
| ATOM | 1995 | CD2 | LEU | 53 | 56.801 | 62.143 | 21.785 | 1.00 | 21.02 | B_13 |
| ATOM | 1996 | C | LEU | 53 | 60.657 | 60.944 | 19.813 | 1.00 | 15.08 | B_13 |
| ATOM | 1997 | O | LEU | 53 | 60.822 | 60.539 | 18.671 | 1.00 | 13.89 | B_13 |
| ATOM | 1998 | N | HIS | 54 | 61.532 | 60.750 | 20.792 | 1.00 | 19.96 | B_13 |
| ATOM | 2000 | CA | HIS | 54 | 62.812 | 60.079 | 20.568 | 1.00 | 28.80 | B_13 |
| ATOM | 2001 | CB | HIS | 54 | 63.848 | 60.604 | 21.569 | 1.00 | 19.40 | B_13 |
| ATOM | 2002 | CG | HIS | 54 | 64.113 | 62.075 | 21.431 | 1.00 | 31.96 | B_13 |
| ATOM | 2003 | CD2 | HIS | 54 | 63.365 | 63.060 | 20.883 | 1.00 | 21.32 | B_13 |
| ATOM | 2004 | ND1 | HIS | 54 | 65.292 | 62.662 | 21.835 | 1.00 | 33.94 | B_13 |
| ATOM | 2006 | CE1 | HIS | 54 | 65.260 | 63.949 | 21.539 | 1.00 | 18.64 | B_13 |
| ATOM | 2007 | NE2 | HIS | 54 | 64.103 | 64.218 | 20.960 | 1.00 | 19.56 | B_13 |

59/75

| | | | | | | | | | | |
|------|------|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 2009 | C | HIS | 54 | 62.695 | 58.555 | 20.647 | 1.00 | 13.04 | B_13 |
| ATOM | 2010 | O | HIS | 54 | 63.620 | 57.850 | 20.282 | 1.00 | 19.90 | B_13 |
| ATOM | 2011 | N | ASP | 55 | 61.586 | 58.076 | 21.219 | 1.00 | 17.27 | B_13 |
| ATOM | 2013 | CA | ASP | 55 | 61.303 | 56.648 | 21.366 | 1.00 | 25.79 | B_13 |
| ATOM | 2014 | CB | ASP | 55 | 62.099 | 56.038 | 22.533 | 1.00 | 29.40 | B_13 |
| ATOM | 2015 | CG | ASP | 55 | 63.443 | 55.428 | 22.076 | 1.00 | 29.64 | B_13 |
| ATOM | 2016 | OD1 | ASP | 55 | 63.517 | 54.906 | 20.942 | 1.00 | 33.28 | B_13 |
| ATOM | 2017 | OD2 | ASP | 55 | 64.437 | 55.469 | 22.831 | 1.00 | 31.99 | B_13 |
| ATOM | 2018 | C | ASP | 55 | 59.807 | 56.460 | 21.567 | 1.00 | 24.99 | B_13 |
| ATOM | 2019 | O | ASP | 55 | 59.079 | 57.445 | 21.677 | 1.00 | 21.06 | B_13 |
| ATOM | 2020 | N | GLY | 56 | 59.358 | 55.207 | 21.559 | 1.00 | 22.90 | B_13 |
| ATOM | 2022 | CA | GLY | 56 | 57.954 | 54.877 | 21.737 | 1.00 | 21.80 | B_13 |
| ATOM | 2023 | C | GLY | 56 | 57.155 | 54.926 | 20.447 | 1.00 | 14.48 | B_13 |
| ATOM | 2024 | O | GLY | 56 | 57.720 | 55.108 | 19.379 | 1.00 | 19.38 | B_13 |
| ATOM | 2025 | N | ILE | 57 | 55.841 | 54.742 | 20.545 | 1.00 | 11.78 | B_13 |
| ATOM | 2027 | CA | ILE | 57 | 54.944 | 54.809 | 19.389 | 1.00 | 16.25 | B_13 |
| ATOM | 2028 | CB | ILE | 57 | 53.737 | 53.804 | 19.510 | 1.00 | 22.94 | B_13 |
| ATOM | 2029 | CG2 | ILE | 57 | 52.442 | 54.417 | 18.955 | 1.00 | 24.79 | B_13 |
| ATOM | 2030 | CG1 | ILE | 57 | 54.025 | 52.505 | 18.744 | 1.00 | 25.63 | B_13 |
| ATOM | 2031 | CD1 | ILE | 57 | 53.586 | 52.520 | 17.240 | 1.00 | 17.48 | B_13 |
| ATOM | 2032 | C | ILE | 57 | 54.410 | 56.238 | 19.301 | 1.00 | 18.78 | B_13 |
| ATOM | 2033 | O | ILE | 57 | 53.866 | 56.777 | 20.270 | 1.00 | 11.40 | B_13 |
| ATOM | 2034 | N | ALA | 58 | 54.598 | 56.842 | 18.140 | 1.00 | 14.67 | B_13 |
| ATOM | 2036 | CA | ALA | 58 | 54.139 | 58.200 | 17.857 | 1.00 | 17.04 | B_13 |
| ATOM | 2037 | CB | ALA | 58 | 55.270 | 59.015 | 17.245 | 1.00 | 10.00 | B_13 |
| ATOM | 2038 | C | ALA | 58 | 53.048 | 58.009 | 16.825 | 1.00 | 25.41 | B_13 |
| ATOM | 2039 | O | ALA | 58 | 52.956 | 56.940 | 16.243 | 1.00 | 22.59 | B_13 |
| ATOM | 2040 | N | ASP | 59 | 52.211 | 59.020 | 16.609 | 1.00 | 13.36 | B_13 |
| ATOM | 2042 | CA | ASP | 59 | 51.156 | 58.927 | 15.606 | 1.00 | 24.67 | B_13 |
| ATOM | 2043 | CB | ASP | 59 | 50.348 | 60.237 | 15.545 | 1.00 | 10.00 | B_13 |
| ATOM | 2044 | CG | ASP | 59 | 49.743 | 60.631 | 16.899 | 1.00 | 12.93 | B_13 |
| ATOM | 2045 | OD1 | ASP | 59 | 49.922 | 61.788 | 17.327 | 1.00 | 32.89 | B_13 |
| ATOM | 2046 | OD2 | ASP | 59 | 49.076 | 59.793 | 17.541 | 1.00 | 21.52 | B_13 |
| ATOM | 2047 | C | ASP | 59 | 51.784 | 58.653 | 14.242 | 1.00 | 11.46 | B_13 |
| ATOM | 2048 | O | ASP | 59 | 51.378 | 57.736 | 13.531 | 1.00 | 16.58 | B_13 |
| ATOM | 2049 | N | ILE | 60 | 52.791 | 59.445 | 13.899 | 1.00 | 24.90 | B_13 |
| ATOM | 2051 | CA | ILE | 60 | 53.494 | 59.346 | 12.624 | 1.00 | 12.17 | B_13 |
| ATOM | 2052 | CB | ILE | 60 | 53.620 | 60.738 | 11.975 | 1.00 | 10.91 | B_13 |
| ATOM | 2053 | CG2 | ILE | 60 | 54.289 | 60.641 | 10.588 | 1.00 | 10.70 | B_13 |
| ATOM | 2054 | CG1 | ILE | 60 | 52.228 | 61.367 | 11.851 | 1.00 | 18.58 | B_13 |
| ATOM | 2055 | CD1 | ILE | 60 | 52.219 | 62.870 | 11.726 | 1.00 | 12.00 | B_13 |
| ATOM | 2056 | C | ILE | 60 | 54.881 | 58.750 | 12.841 | 1.00 | 12.93 | B_13 |
| ATOM | 2057 | O | ILE | 60 | 55.788 | 59.392 | 13.365 | 1.00 | 16.39 | B_13 |
| ATOM | 2058 | N | MET | 61 | 55.015 | 57.485 | 12.483 | 1.00 | 19.08 | B_13 |
| ATOM | 2060 | CA | MET | 61 | 56.275 | 56.784 | 12.617 | 1.00 | 16.97 | B_13 |
| ATOM | 2061 | CB | MET | 61 | 56.011 | 55.328 | 13.035 | 1.00 | 23.79 | B_13 |
| ATOM | 2062 | CG | MET | 61 | 55.313 | 55.172 | 14.422 | 1.00 | 12.37 | B_13 |
| ATOM | 2063 | SD | MET | 61 | 56.389 | 55.360 | 15.913 | 1.00 | 31.01 | B_13 |
| ATOM | 2064 | CE | MET | 61 | 57.204 | 53.749 | 15.861 | 1.00 | 14.93 | B_13 |
| ATOM | 2065 | C | MET | 61 | 56.995 | 56.888 | 11.265 | 1.00 | 12.72 | B_13 |
| ATOM | 2066 | O | MET | 61 | 56.438 | 56.538 | 10.216 | 1.00 | 15.31 | B_13 |
| ATOM | 2067 | N | ILE | 62 | 58.170 | 57.518 | 11.294 | 1.00 | 16.64 | B_13 |
| ATOM | 2069 | CA | ILE | 62 | 58.978 | 57.739 | 10.097 | 1.00 | 27.48 | B_13 |
| ATOM | 2070 | CB | ILE | 62 | 59.557 | 59.181 | 10.060 | 1.00 | 10.00 | B_13 |
| ATOM | 2071 | CG2 | ILE | 62 | 60.191 | 59.462 | 8.717 | 1.00 | 18.65 | B_13 |
| ATOM | 2072 | CG1 | ILE | 62 | 58.460 | 60.203 | 10.342 | 1.00 | 18.51 | B_13 |
| ATOM | 2073 | CD1 | ILE | 62 | 58.983 | 61.499 | 10.931 | 1.00 | 16.23 | B_13 |
| ATOM | 2074 | C | ILE | 62 | 60.155 | 56.787 | 10.046 | 1.00 | 15.06 | B_13 |
| ATOM | 2075 | O | ILE | 62 | 60.873 | 56.606 | 11.033 | 1.00 | 10.73 | B_13 |
| ATOM | 2076 | N | SER | 63 | 60.398 | 56.230 | 8.873 | 1.00 | 19.40 | B_13 |
| ATOM | 2078 | CA | SER | 63 | 61.513 | 55.321 | 8.722 | 1.00 | 13.31 | B_13 |
| ATOM | 2079 | CB | SER | 63 | 61.111 | 53.888 | 9.123 | 1.00 | 17.28 | B_13 |
| ATOM | 2080 | OG | SER | 63 | 59.985 | 53.435 | 8.391 | 1.00 | 13.66 | B_13 |
| ATOM | 2082 | C | SER | 63 | 62.086 | 55.339 | 7.315 | 1.00 | 19.86 | B_13 |
| ATOM | 2083 | O | SER | 63 | 61.441 | 55.766 | 6.347 | 1.00 | 20.93 | B_13 |
| ATOM | 2084 | N | PHE | 64 | 63.338 | 54.914 | 7.237 | 1.00 | 17.78 | B_13 |
| ATOM | 2086 | CA | PHE | 64 | 64.072 | 54.823 | 5.989 | 1.00 | 18.81 | B_13 |
| ATOM | 2087 | CB | PHE | 64 | 65.409 | 55.553 | 6.105 | 1.00 | 16.50 | B_13 |
| ATOM | 2088 | CG | PHE | 64 | 65.278 | 57.054 | 6.171 | 1.00 | 22.54 | B_13 |
| ATOM | 2089 | CD1 | PHE | 64 | 65.321 | 57.817 | 5.013 | 1.00 | 20.48 | B_13 |
| ATOM | 2090 | CD2 | PHE | 64 | 65.155 | 57.708 | 7.395 | 1.00 | 24.76 | B_13 |
| ATOM | 2091 | CE1 | PHE | 64 | 65.246 | 59.207 | 5.071 | 1.00 | 13.94 | B_13 |
| ATOM | 2092 | CE2 | PHE | 64 | 65.079 | 59.105 | 7.461 | 1.00 | 14.29 | B_13 |
| ATOM | 2093 | CZ | PHE | 64 | 65.128 | 59.847 | 6.298 | 1.00 | 10.16 | B_13 |
| ATOM | 2094 | C | PHE | 64 | 64.293 | 53.336 | 5.823 | 1.00 | 10.30 | B_13 |
| ATOM | 2095 | O | PHE | 64 | 64.571 | 52.637 | 6.799 | 1.00 | 14.11 | B_13 |
| ATOM | 2096 | N | GLY | 65 | 64.121 | 52.842 | 4.610 | 1.00 | 13.58 | B_13 |

60/75

| | | | | | | | | | | |
|------|------|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 2098 | CA | GLY | 65 | 64.306 | 51.426 | 4.392 | 1.00 | 14.88 | B_13 |
| ATOM | 2099 | C | GLY | 65 | 64.400 | 51.117 | 2.922 | 1.00 | 14.95 | B_13 |
| ATOM | 2100 | O | GLY | 65 | 64.047 | 51.947 | 2.088 | 1.00 | 12.61 | B_13 |
| ATOM | 2101 | N | ILE | 66 | 64.860 | 49.922 | 2.587 | 1.00 | 10.00 | B_13 |
| ATOM | 2103 | CA | ILE | 66 | 64.995 | 49.555 | 1.187 | 1.00 | 19.70 | B_13 |
| ATOM | 2104 | CB | ILE | 66 | 66.483 | 49.344 | 0.791 | 1.00 | 18.92 | B_13 |
| ATOM | 2105 | CG2 | ILE | 66 | 67.301 | 50.628 | 1.073 | 1.00 | 10.00 | B_13 |
| ATOM | 2106 | CG1 | ILE | 66 | 67.078 | 48.178 | 1.582 | 1.00 | 14.64 | B_13 |
| ATOM | 2107 | CD1 | ILE | 66 | 68.381 | 47.662 | 1.004 | 1.00 | 17.53 | B_13 |
| ATOM | 2108 | C | ILE | 66 | 64.195 | 48.296 | 0.900 | 1.00 | 15.98 | B_13 |
| ATOM | 2109 | O | ILE | 66 | 63.877 | 47.543 | 1.806 | 1.00 | 20.10 | B_13 |
| ATOM | 2110 | N | LYS | 67 | 63.773 | 48.148 | -0.349 | 1.00 | 18.78 | B_13 |
| ATOM | 2112 | CA | LYS | 67 | 63.019 | 46.980 | -0.787 | 1.00 | 14.73 | B_13 |
| ATOM | 2113 | CB | LYS | 67 | 63.986 | 45.827 | -1.073 | 1.00 | 22.08 | B_13 |
| ATOM | 2114 | CG | LYS | 67 | 65.107 | 46.142 | -2.066 | 1.00 | 15.53 | B_13 |
| ATOM | 2115 | CD | LYS | 67 | 64.591 | 46.325 | -3.487 | 1.00 | 16.76 | B_13 |
| ATOM | 2116 | CE | LYS | 67 | 65.573 | 45.763 | -4.523 | 1.00 | 21.90 | B_13 |
| ATOM | 2117 | NZ | LYS | 67 | 66.975 | 46.257 | -4.394 | 1.00 | 28.03 | B_13 |
| ATOM | 2121 | C | LYS | 67 | 61.945 | 46.548 | 0.218 | 1.00 | 16.24 | B_13 |
| ATOM | 2122 | O | LYS | 67 | 61.136 | 47.360 | 0.649 | 1.00 | 10.25 | B_13 |
| ATOM | 2123 | N | GLU | 68 | 61.968 | 45.293 | 0.630 | 1.00 | 10.00 | B_13 |
| ATOM | 2125 | CA | GLU | 68 | 60.986 | 44.787 | 1.570 | 1.00 | 10.00 | B_13 |
| ATOM | 2126 | CB | GLU | 68 | 61.004 | 43.257 | 1.505 | 1.00 | 31.44 | B_13 |
| ATOM | 2127 | CG | GLU | 68 | 59.733 | 42.550 | 1.696 | 1.00 | 27.13 | B_13 |
| ATOM | 2128 | CD | GLU | 68 | 58.723 | 42.720 | 0.524 | 1.00 | 12.88 | B_13 |
| ATOM | 2129 | OE1 | GLU | 68 | 59.106 | 42.180 | -0.613 | 1.00 | 14.05 | B_13 |
| ATOM | 2130 | OE2 | GLU | 68 | 57.681 | 43.274 | 0.753 | 1.00 | 38.61 | B_13 |
| ATOM | 2131 | C | GLU | 68 | 61.402 | 45.292 | 2.954 | 1.00 | 32.89 | B_13 |
| ATOM | 2132 | O | GLU | 68 | 62.541 | 45.099 | 3.390 | 1.00 | 19.77 | B_13 |
| ATOM | 2133 | N | HIS | 69 | 60.467 | 45.918 | 3.659 | 1.00 | 15.43 | B_13 |
| ATOM | 2135 | CA | HIS | 69 | 60.777 | 46.473 | 4.964 | 1.00 | 10.00 | B_13 |
| ATOM | 2136 | CB | HIS | 69 | 61.173 | 47.928 | 4.802 | 1.00 | 15.60 | B_13 |
| ATOM | 2137 | CG | HIS | 69 | 60.151 | 48.731 | 4.063 | 1.00 | 18.06 | B_13 |
| ATOM | 2138 | CD2 | HIS | 69 | 59.131 | 49.509 | 4.498 | 1.00 | 25.01 | B_13 |
| ATOM | 2139 | ND1 | HIS | 69 | 60.055 | 48.709 | 2.689 | 1.00 | 21.79 | B_13 |
| ATOM | 2141 | CE1 | HIS | 69 | 59.023 | 49.430 | 2.308 | 1.00 | 19.43 | B_13 |
| ATOM | 2142 | NE2 | HIS | 69 | 58.438 | 49.932 | 3.384 | 1.00 | 19.23 | B_13 |
| ATOM | 2143 | C | HIS | 69 | 59.655 | 46.396 | 5.978 | 1.00 | 16.27 | B_13 |
| ATOM | 2144 | O | HIS | 69 | 59.689 | 47.099 | 6.969 | 1.00 | 13.47 | B_13 |
| ATOM | 2145 | N | GLY | 70 | 58.610 | 45.629 | 5.719 | 1.00 | 21.21 | B_13 |
| ATOM | 2147 | CA | GLY | 70 | 57.567 | 45.520 | 6.720 | 1.00 | 15.93 | B_13 |
| ATOM | 2148 | C | GLY | 70 | 56.147 | 45.784 | 6.287 | 1.00 | 13.13 | B_13 |
| ATOM | 2149 | O | GLY | 70 | 55.283 | 45.986 | 7.147 | 1.00 | 12.19 | B_13 |
| ATOM | 2150 | N | ASP | 71 | 55.891 | 45.805 | 4.983 | 1.00 | 10.00 | B_13 |
| ATOM | 2152 | CA | ASP | 71 | 54.540 | 46.030 | 4.480 | 1.00 | 17.84 | B_13 |
| ATOM | 2153 | CB | ASP | 71 | 54.086 | 47.490 | 4.636 | 1.00 | 21.86 | B_13 |
| ATOM | 2154 | CG | ASP | 71 | 54.946 | 48.480 | 3.881 | 1.00 | 13.38 | B_13 |
| ATOM | 2155 | OD1 | ASP | 71 | 54.896 | 49.644 | 4.291 | 1.00 | 10.00 | B_13 |
| ATOM | 2156 | OD2 | ASP | 71 | 55.633 | 48.135 | 2.897 | 1.00 | 10.00 | B_13 |
| ATOM | 2157 | C | ASP | 71 | 54.313 | 45.557 | 3.064 | 1.00 | 27.18 | B_13 |
| ATOM | 2158 | O | ASP | 71 | 55.221 | 45.068 | 2.416 | 1.00 | 16.61 | B_13 |
| ATOM | 2159 | N | PHE | 72 | 53.103 | 45.759 | 2.564 | 1.00 | 10.00 | B_13 |
| ATOM | 2161 | CA | PHE | 72 | 52.788 | 45.317 | 1.213 | 1.00 | 19.60 | B_13 |
| ATOM | 2162 | CB | PHE | 72 | 51.292 | 45.017 | 1.099 | 1.00 | 16.43 | B_13 |
| ATOM | 2163 | CG | PHE | 72 | 50.849 | 43.779 | 1.851 | 1.00 | 27.69 | B_13 |
| ATOM | 2164 | CD1 | PHE | 72 | 51.399 | 42.532 | 1.561 | 1.00 | 22.33 | B_13 |
| ATOM | 2165 | CD2 | PHE | 72 | 49.848 | 43.855 | 2.823 | 1.00 | 27.58 | B_13 |
| ATOM | 2166 | CE1 | PHE | 72 | 50.955 | 41.383 | 2.225 | 1.00 | 22.03 | B_13 |
| ATOM | 2167 | CE2 | PHE | 72 | 49.403 | 42.709 | 3.486 | 1.00 | 21.82 | B_13 |
| ATOM | 2168 | CZ | PHE | 72 | 49.957 | 41.473 | 3.184 | 1.00 | 10.00 | B_13 |
| ATOM | 2169 | C | PHE | 72 | 53.225 | 46.313 | 0.130 | 1.00 | 18.56 | B_13 |
| ATOM | 2170 | O | PHE | 72 | 52.840 | 46.190 | -1.048 | 1.00 | 14.78 | B_13 |
| ATOM | 2171 | N | TYR | 73 | 54.079 | 47.260 | 0.513 | 1.00 | 10.93 | B_13 |
| ATOM | 2173 | CA | TYR | 73 | 54.558 | 48.295 | -0.416 | 1.00 | 13.87 | B_13 |
| ATOM | 2174 | CB | TYR | 73 | 53.943 | 49.649 | -0.048 | 1.00 | 22.69 | B_13 |
| ATOM | 2175 | CG | TYR | 73 | 52.439 | 49.581 | 0.007 | 1.00 | 16.43 | B_13 |
| ATOM | 2176 | CD1 | TYR | 73 | 51.774 | 49.385 | 1.219 | 1.00 | 18.21 | B_13 |
| ATOM | 2177 | CE1 | TYR | 73 | 50.386 | 49.219 | 1.257 | 1.00 | 35.13 | B_13 |
| ATOM | 2178 | CD2 | TYR | 73 | 51.683 | 49.618 | -1.165 | 1.00 | 15.77 | B_13 |
| ATOM | 2179 | CE2 | TYR | 73 | 50.300 | 49.456 | -1.133 | 1.00 | 39.16 | B_13 |
| ATOM | 2180 | CZ | TYR | 73 | 49.663 | 49.258 | 0.080 | 1.00 | 28.27 | B_13 |
| ATOM | 2181 | OH | TYR | 73 | 48.301 | 49.122 | 0.106 | 1.00 | 33.06 | B_13 |
| ATOM | 2183 | C | TYR | 73 | 56.088 | 48.349 | -0.425 | 1.00 | 18.05 | B_13 |
| ATOM | 2184 | O | TYR | 73 | 56.721 | 49.339 | 0.003 | 1.00 | 10.00 | B_13 |
| ATOM | 2185 | N | PRO | 74 | 56.702 | 47.287 | -0.953 | 1.00 | 13.76 | B_13 |
| ATOM | 2186 | CD | PRO | 74 | 56.063 | 46.221 | -1.740 | 1.00 | 14.21 | B_13 |
| ATOM | 2187 | CA | PRO | 74 | 58.158 | 47.183 | -1.024 | 1.00 | 21.66 | B_13 |

61/75

| | | | | | | | | | | |
|------|------|-----|-----|----|--------|--------|---------|------|-------|------|
| ATOM | 2188 | CB | PRO | 74 | 58.353 | 45.768 | -1.569 | 1.00 | 15.88 | B_13 |
| ATOM | 2189 | CG | PRO | 74 | 57.225 | 45.653 | -2.540 | 1.00 | 13.95 | B_13 |
| ATOM | 2190 | C | PRO | 74 | 58.747 | 48.226 | -1.959 | 1.00 | 27.68 | B_13 |
| ATOM | 2191 | O | PRO | 74 | 58.173 | 48.526 | -3.012 | 1.00 | 21.90 | B_13 |
| ATOM | 2192 | N | PHE | 75 | 59.883 | 48.794 | -1.562 | 1.00 | 20.91 | B_13 |
| ATOM | 2194 | CA | PHE | 75 | 60.554 | 49.773 | -2.395 | 1.00 | 15.84 | B_13 |
| ATOM | 2195 | CB | PHE | 75 | 61.498 | 50.637 | -1.548 | 1.00 | 11.67 | B_13 |
| ATOM | 2196 | CG | PHE | 75 | 60.765 | 51.589 | -0.641 | 1.00 | 14.42 | B_13 |
| ATOM | 2197 | CD1 | PHE | 75 | 59.831 | 52.484 | -1.162 | 1.00 | 16.56 | B_13 |
| ATOM | 2198 | CD2 | PHE | 75 | 60.976 | 51.574 | 0.726 | 1.00 | 10.00 | B_13 |
| ATOM | 2199 | CE1 | PHE | 75 | 59.119 | 53.345 | -0.327 | 1.00 | 11.14 | B_13 |
| ATOM | 2200 | CE2 | PHE | 75 | 60.274 | 52.423 | 1.558 | 1.00 | 10.28 | B_13 |
| ATOM | 2201 | CZ | PHE | 75 | 59.340 | 53.316 | 1.027 | 1.00 | 10.00 | B_13 |
| ATOM | 2202 | C | PHE | 75 | 61.236 | 49.068 | -3.573 | 1.00 | 14.23 | B_13 |
| ATOM | 2203 | O | PHE | 75 | 61.357 | 47.837 | -3.582 | 1.00 | 18.64 | B_13 |
| ATOM | 2204 | N | ASP | 76 | 61.742 | 49.845 | -4.526 | 1.00 | 12.83 | B_13 |
| ATOM | 2206 | CA | ASP | 76 | 62.330 | 49.287 | -5.740 | 1.00 | 20.69 | B_13 |
| ATOM | 2207 | CB | ASP | 76 | 61.394 | 49.644 | -6.911 | 1.00 | 14.28 | B_13 |
| ATOM | 2208 | CG | ASP | 76 | 61.212 | 51.144 | -7.080 | 1.00 | 14.37 | B_13 |
| ATOM | 2209 | OD1 | ASP | 76 | 61.361 | 51.882 | -6.095 | 1.00 | 22.32 | B_13 |
| ATOM | 2210 | OD2 | ASP | 76 | 60.941 | 51.597 | -8.202 | 1.00 | 15.92 | B_13 |
| ATOM | 2211 | C | ASP | 76 | 63.764 | 49.698 | -6.104 | 1.00 | 19.31 | B_13 |
| ATOM | 2212 | O | ASP | 76 | 64.056 | 49.864 | -7.278 | 1.00 | 18.67 | B_13 |
| ATOM | 2213 | N | GLY | 77 | 64.653 | 49.902 | -5.132 | 1.00 | 10.00 | B_13 |
| ATOM | 2215 | CA | GLY | 77 | 65.997 | 50.326 | -5.501 | 1.00 | 10.00 | B_13 |
| ATOM | 2216 | C | GLY | 77 | 65.989 | 51.790 | -5.970 | 1.00 | 16.22 | B_13 |
| ATOM | 2217 | O | GLY | 77 | 64.967 | 52.487 | -5.752 | 1.00 | 17.04 | B_13 |
| ATOM | 2218 | N | PRO | 78 | 67.080 | 52.305 | -6.589 | 1.00 | 12.53 | B_13 |
| ATOM | 2219 | CD | PRO | 78 | 68.319 | 51.564 | -6.856 | 1.00 | 12.24 | B_13 |
| ATOM | 2220 | CA | PRO | 78 | 67.207 | 53.691 | -7.086 | 1.00 | 11.81 | B_13 |
| ATOM | 2221 | CB | PRO | 78 | 68.546 | 53.678 | -7.816 | 1.00 | 10.00 | B_13 |
| ATOM | 2222 | CG | PRO | 78 | 69.316 | 52.693 | -7.066 | 1.00 | 12.78 | B_13 |
| ATOM | 2223 | C | PRO | 78 | 66.093 | 54.146 | -8.027 | 1.00 | 10.00 | B_13 |
| ATOM | 2224 | O | PRO | 78 | 65.621 | 53.381 | -8.853 | 1.00 | 27.46 | B_13 |
| ATOM | 2225 | N | SER | 79 | 65.641 | 55.386 | -7.852 | 1.00 | 19.14 | B_13 |
| ATOM | 2227 | CA | SER | 79 | 64.568 | 55.963 | -8.669 | 1.00 | 10.00 | B_13 |
| ATOM | 2228 | CB | SER | 79 | 64.970 | 56.033 | -10.148 | 1.00 | 20.11 | B_13 |
| ATOM | 2229 | OG | SER | 79 | 63.982 | 56.723 | -10.901 | 1.00 | 23.87 | B_13 |
| ATOM | 2231 | C | SER | 79 | 63.231 | 55.215 | -8.507 | 1.00 | 31.68 | B_13 |
| ATOM | 2232 | O | SER | 79 | 63.074 | 54.356 | -7.606 | 1.00 | 26.48 | B_13 |
| ATOM | 2233 | N | GLY | 80 | 62.250 | 55.589 | -9.327 | 1.00 | 10.00 | B_13 |
| ATOM | 2235 | CA | GLY | 80 | 60.940 | 54.969 | -9.260 | 1.00 | 10.07 | B_13 |
| ATOM | 2236 | C | GLY | 80 | 60.293 | 55.412 | -7.968 | 1.00 | 30.72 | B_13 |
| ATOM | 2237 | O | GLY | 80 | 60.347 | 56.600 | -7.643 | 1.00 | 20.65 | B_13 |
| ATOM | 2238 | N | LEU | 81 | 59.779 | 54.452 | -7.193 | 1.00 | 23.74 | B_13 |
| ATOM | 2240 | CA | LEU | 81 | 59.135 | 54.752 | -5.917 | 1.00 | 13.14 | B_13 |
| ATOM | 2241 | CB | LEU | 81 | 58.661 | 53.481 | -5.213 | 1.00 | 16.20 | B_13 |
| ATOM | 2242 | CG | LEU | 81 | 57.393 | 52.775 | -5.687 | 1.00 | 17.33 | B_13 |
| ATOM | 2243 | CD1 | LEU | 81 | 57.554 | 52.277 | -7.096 | 1.00 | 28.67 | B_13 |
| ATOM | 2244 | CD2 | LEU | 81 | 57.103 | 51.617 | -4.745 | 1.00 | 27.02 | B_13 |
| ATOM | 2245 | C | LEU | 81 | 60.122 | 55.466 | -5.019 | 1.00 | 14.51 | B_13 |
| ATOM | 2246 | O | LEU | 81 | 61.264 | 55.016 | -4.846 | 1.00 | 16.24 | B_13 |
| ATOM | 2247 | N | LEU | 82 | 59.692 | 56.590 | -4.470 | 1.00 | 11.33 | B_13 |
| ATOM | 2249 | CA | LEU | 82 | 60.540 | 57.381 | -3.594 | 1.00 | 17.52 | B_13 |
| ATOM | 2250 | CB | LEU | 82 | 60.442 | 58.861 | -3.986 | 1.00 | 18.51 | B_13 |
| ATOM | 2251 | CG | LEU | 82 | 61.355 | 59.499 | -5.044 | 1.00 | 15.37 | B_13 |
| ATOM | 2252 | CD1 | LEU | 82 | 61.800 | 58.504 | -6.104 | 1.00 | 17.05 | B_13 |
| ATOM | 2253 | CD2 | LEU | 82 | 60.639 | 60.744 | -5.659 | 1.00 | 16.87 | B_13 |
| ATOM | 2254 | C | LEU | 82 | 60.172 | 57.203 | -2.127 | 1.00 | 10.00 | B_13 |
| ATOM | 2255 | O | LEU | 82 | 61.045 | 57.056 | -1.275 | 1.00 | 19.90 | B_13 |
| ATOM | 2256 | N | ALA | 83 | 58.876 | 57.201 | -1.840 | 1.00 | 18.16 | B_13 |
| ATOM | 2258 | CA | ALA | 83 | 58.378 | 57.077 | -0.472 | 1.00 | 13.17 | B_13 |
| ATOM | 2259 | CB | ALA | 83 | 58.762 | 58.322 | 0.327 | 1.00 | 10.00 | B_13 |
| ATOM | 2260 | C | ALA | 83 | 56.846 | 56.925 | -0.500 | 1.00 | 10.00 | B_13 |
| ATOM | 2261 | O | ALA | 83 | 56.209 | 57.155 | -1.541 | 1.00 | 10.73 | B_13 |
| ATOM | 2262 | N | HIS | 84 | 56.268 | 56.619 | 0.662 | 1.00 | 10.00 | B_13 |
| ATOM | 2264 | CA | HIS | 84 | 54.811 | 56.472 | 0.810 | 1.00 | 23.81 | B_13 |
| ATOM | 2265 | CB | HIS | 84 | 54.270 | 55.188 | 0.157 | 1.00 | 30.45 | B_13 |
| ATOM | 2266 | CG | HIS | 84 | 54.848 | 53.925 | 0.711 | 1.00 | 17.68 | B_13 |
| ATOM | 2267 | CD2 | HIS | 84 | 54.856 | 53.415 | 1.964 | 1.00 | 10.00 | B_13 |
| ATOM | 2268 | ND1 | HIS | 84 | 55.525 | 53.025 | -0.076 | 1.00 | 14.94 | B_13 |
| ATOM | 2270 | CE1 | HIS | 84 | 55.933 | 52.015 | 0.666 | 1.00 | 29.72 | B_13 |
| ATOM | 2271 | NE2 | HIS | 84 | 55.543 | 52.224 | 1.912 | 1.00 | 13.81 | B_13 |
| ATOM | 2272 | C | HIS | 84 | 54.363 | 56.547 | 2.258 | 1.00 | 12.82 | B_13 |
| ATOM | 2273 | O | HIS | 84 | 55.099 | 56.148 | 3.166 | 1.00 | 20.02 | B_13 |
| ATOM | 2274 | N | ALA | 85 | 53.161 | 57.076 | 2.464 | 1.00 | 28.38 | B_13 |
| ATOM | 2276 | CA | ALA | 85 | 52.584 | 57.230 | 3.796 | 1.00 | 18.64 | B_13 |

62/75

| | | | | | | | | | | |
|------|------|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 2277 | CB | ALA | 85 | 52.638 | 58.705 | 4.223 | 1.00 | 13.89 | B_13 |
| ATOM | 2278 | C | ALA | 85 | 51.138 | 56.716 | 3.837 | 1.00 | 10.00 | B_13 |
| ATOM | 2279 | O | ALA | 85 | 50.434 | 56.728 | 2.828 | 1.00 | 10.00 | B_13 |
| ATOM | 2280 | N | PHE | 86 | 50.676 | 56.322 | 5.016 | 1.00 | 14.76 | B_13 |
| ATOM | 2282 | CA | PHE | 86 | 49.316 | 55.811 | 5.143 | 1.00 | 17.96 | B_13 |
| ATOM | 2283 | CB | PHE | 86 | 49.286 | 54.592 | 6.084 | 1.00 | 15.86 | B_13 |
| ATOM | 2284 | CG | PHE | 86 | 50.320 | 53.542 | 5.748 | 1.00 | 26.30 | B_13 |
| ATOM | 2285 | CD1 | PHE | 86 | 49.973 | 52.398 | 5.042 | 1.00 | 22.30 | B_13 |
| ATOM | 2286 | CD2 | PHE | 86 | 51.654 | 53.730 | 6.090 | 1.00 | 27.63 | B_13 |
| ATOM | 2287 | CE1 | PHE | 86 | 50.938 | 51.472 | 4.681 | 1.00 | 27.85 | B_13 |
| ATOM | 2288 | CE2 | PHE | 86 | 52.620 | 52.810 | 5.731 | 1.00 | 13.97 | B_13 |
| ATOM | 2289 | CZ | PHE | 86 | 52.266 | 51.683 | 5.027 | 1.00 | 23.08 | B_13 |
| ATOM | 2290 | C | PHE | 86 | 48.427 | 56.924 | 5.669 | 1.00 | 13.02 | B_13 |
| ATOM | 2291 | O | PHE | 86 | 48.870 | 57.747 | 6.466 | 1.00 | 15.02 | B_13 |
| ATOM | 2292 | N | PRO | 87 | 47.174 | 57.006 | 5.186 | 1.00 | 17.55 | B_13 |
| ATOM | 2293 | CD | PRO | 87 | 46.565 | 56.165 | 4.146 | 1.00 | 10.17 | B_13 |
| ATOM | 2294 | CA | PRO | 87 | 46.228 | 58.041 | 5.628 | 1.00 | 32.09 | B_13 |
| ATOM | 2295 | CB | PRO | 87 | 44.961 | 57.720 | 4.819 | 1.00 | 18.55 | B_13 |
| ATOM | 2296 | CG | PRO | 87 | 45.115 | 56.277 | 4.481 | 1.00 | 18.86 | B_13 |
| ATOM | 2297 | C | PRO | 87 | 45.995 | 57.955 | 7.139 | 1.00 | 25.18 | B_13 |
| ATOM | 2298 | O | PRO | 87 | 46.284 | 56.919 | 7.752 | 1.00 | 18.18 | B_13 |
| ATOM | 2299 | N | PRO | 88 | 45.462 | 59.032 | 7.760 | 1.00 | 11.49 | B_13 |
| ATOM | 2300 | CD | PRO | 88 | 45.015 | 60.303 | 7.164 | 1.00 | 10.00 | B_13 |
| ATOM | 2301 | CA | PRO | 88 | 45.217 | 59.034 | 9.202 | 1.00 | 19.03 | B_13 |
| ATOM | 2302 | CB | PRO | 88 | 44.399 | 60.302 | 9.402 | 1.00 | 14.16 | B_13 |
| ATOM | 2303 | CG | PRO | 88 | 44.939 | 61.196 | 8.357 | 1.00 | 16.39 | B_13 |
| ATOM | 2304 | C | PRO | 88 | 44.500 | 57.787 | 9.733 | 1.00 | 25.43 | B_13 |
| ATOM | 2305 | O | PRO | 88 | 43.670 | 57.165 | 9.044 | 1.00 | 15.90 | B_13 |
| ATOM | 2306 | N | GLY | 89 | 44.865 | 57.422 | 10.955 | 1.00 | 26.28 | B_13 |
| ATOM | 2308 | CA | GLY | 89 | 44.299 | 56.264 | 11.606 | 1.00 | 25.32 | B_13 |
| ATOM | 2309 | C | GLY | 89 | 45.343 | 55.713 | 12.546 | 1.00 | 34.38 | B_13 |
| ATOM | 2310 | O | GLY | 89 | 46.485 | 56.164 | 12.498 | 1.00 | 23.28 | B_13 |
| ATOM | 2311 | N | PRO | 90 | 44.977 | 54.774 | 13.437 | 1.00 | 13.87 | B_13 |
| ATOM | 2312 | CD | PRO | 90 | 43.613 | 54.259 | 13.631 | 1.00 | 16.36 | B_13 |
| ATOM | 2313 | CA | PRO | 90 | 45.898 | 54.164 | 14.398 | 1.00 | 10.34 | B_13 |
| ATOM | 2314 | CB | PRO | 90 | 44.963 | 53.360 | 15.300 | 1.00 | 15.93 | B_13 |
| ATOM | 2315 | CG | PRO | 90 | 43.870 | 52.975 | 14.373 | 1.00 | 23.25 | B_13 |
| ATOM | 2316 | C | PRO | 90 | 46.942 | 53.299 | 13.711 | 1.00 | 18.38 | B_13 |
| ATOM | 2317 | O | PRO | 90 | 46.875 | 53.064 | 12.505 | 1.00 | 26.81 | B_13 |
| ATOM | 2318 | N | ASN | 91 | 47.903 | 52.831 | 14.502 | 1.00 | 26.63 | B_13 |
| ATOM | 2320 | CA | ASN | 91 | 49.022 | 52.010 | 14.033 | 1.00 | 21.91 | B_13 |
| ATOM | 2321 | CB | ASN | 91 | 48.740 | 50.500 | 14.081 | 1.00 | 18.89 | B_13 |
| ATOM | 2322 | CG | ASN | 91 | 47.437 | 50.117 | 13.448 | 1.00 | 22.49 | B_13 |
| ATOM | 2323 | OD1 | ASN | 91 | 47.335 | 50.017 | 12.237 | 1.00 | 29.37 | B_13 |
| ATOM | 2324 | ND2 | ASN | 91 | 46.438 | 49.858 | 14.273 | 1.00 | 28.01 | B_13 |
| ATOM | 2327 | C | ASN | 91 | 49.656 | 52.438 | 12.721 | 1.00 | 20.07 | B_13 |
| ATOM | 2328 | O | ASN | 91 | 50.301 | 53.479 | 12.681 | 1.00 | 21.24 | B_13 |
| ATOM | 2329 | N | TYR | 92 | 49.423 | 51.716 | 11.633 | 1.00 | 20.15 | B_13 |
| ATOM | 2331 | CA | TYR | 92 | 50.052 | 52.081 | 10.367 | 1.00 | 18.70 | B_13 |
| ATOM | 2332 | CB | TYR | 92 | 49.905 | 50.953 | 9.344 | 1.00 | 14.48 | B_13 |
| ATOM | 2333 | CG | TYR | 92 | 50.906 | 49.821 | 9.567 | 1.00 | 24.41 | B_13 |
| ATOM | 2334 | CD1 | TYR | 92 | 52.266 | 50.003 | 9.287 | 1.00 | 27.39 | B_13 |
| ATOM | 2335 | CE1 | TYR | 92 | 53.198 | 48.979 | 9.471 | 1.00 | 18.14 | B_13 |
| ATOM | 2336 | CD2 | TYR | 92 | 50.499 | 48.571 | 10.044 | 1.00 | 28.07 | B_13 |
| ATOM | 2337 | CE2 | TYR | 92 | 51.427 | 47.529 | 10.230 | 1.00 | 36.50 | B_13 |
| ATOM | 2338 | CZ | TYR | 92 | 52.778 | 47.741 | 9.940 | 1.00 | 43.64 | B_13 |
| ATOM | 2339 | OH | TYR | 92 | 53.694 | 46.710 | 10.105 | 1.00 | 32.21 | B_13 |
| ATOM | 2341 | C | TYR | 92 | 49.633 | 53.431 | 9.797 | 1.00 | 21.78 | B_13 |
| ATOM | 2342 | O | TYR | 92 | 50.384 | 54.049 | 9.040 | 1.00 | 12.55 | B_13 |
| ATOM | 2343 | N | GLY | 93 | 48.464 | 53.916 | 10.198 | 1.00 | 15.83 | B_13 |
| ATOM | 2345 | CA | GLY | 93 | 48.015 | 55.216 | 9.732 | 1.00 | 11.69 | B_13 |
| ATOM | 2346 | C | GLY | 93 | 48.971 | 56.326 | 10.134 | 1.00 | 18.60 | B_13 |
| ATOM | 2347 | O | GLY | 93 | 49.561 | 56.300 | 11.227 | 1.00 | 22.00 | B_13 |
| ATOM | 2348 | N | GLY | 94 | 49.205 | 57.258 | 9.216 | 1.00 | 10.27 | B_13 |
| ATOM | 2350 | CA | GLY | 94 | 50.099 | 58.365 | 9.492 | 1.00 | 18.36 | B_13 |
| ATOM | 2351 | C | GLY | 94 | 51.567 | 58.061 | 9.234 | 1.00 | 15.54 | B_13 |
| ATOM | 2352 | O | GLY | 94 | 52.334 | 58.967 | 8.938 | 1.00 | 17.55 | B_13 |
| ATOM | 2353 | N | ASP | 95 | 51.977 | 56.801 | 9.351 | 1.00 | 17.69 | B_13 |
| ATOM | 2355 | CA | ASP | 95 | 53.386 | 56.457 | 9.134 | 1.00 | 19.67 | B_13 |
| ATOM | 2356 | CB | ASP | 95 | 53.637 | 54.986 | 9.444 | 1.00 | 15.96 | B_13 |
| ATOM | 2357 | CG | ASP | 95 | 53.346 | 54.634 | 10.900 | 1.00 | 25.37 | B_13 |
| ATOM | 2358 | OD1 | ASP | 95 | 53.627 | 53.484 | 11.297 | 1.00 | 16.05 | B_13 |
| ATOM | 2359 | OD2 | ASP | 95 | 52.835 | 55.488 | 11.656 | 1.00 | 14.66 | B_13 |
| ATOM | 2360 | C | ASP | 95 | 53.896 | 56.808 | 7.733 | 1.00 | 17.15 | B_13 |
| ATOM | 2361 | O | ASP | 95 | 53.162 | 56.711 | 6.746 | 1.00 | 19.09 | B_13 |
| ATOM | 2362 | N | ALA | 96 | 55.166 | 57.198 | 7.662 | 1.00 | 18.71 | B_13 |
| ATOM | 2364 | CA | ALA | 96 | 55.803 | 57.581 | 6.400 | 1.00 | 19.97 | B_13 |

63/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2365 | CB | ALA | 96 | 56.098 | 59.095 | 6.379 | 1.00 | 22.61 | B_13 |
| ATOM | 2366 | C | ALA | 96 | 57.088 | 56.784 | 6.204 | 1.00 | 25.63 | B_13 |
| ATOM | 2367 | O | ALA | 96 | 57.948 | 56.724 | 7.095 | 1.00 | 12.54 | B_13 |
| ATOM | 2368 | N | HIS | 97 | 57.211 | 56.166 | 5.035 | 1.00 | 13.27 | B_13 |
| ATOM | 2370 | CA | HIS | 97 | 58.375 | 55.357 | 4.730 | 1.00 | 25.28 | B_13 |
| ATOM | 2371 | CB | HIS | 97 | 57.955 | 53.905 | 4.464 | 1.00 | 10.00 | B_13 |
| ATOM | 2372 | CG | HIS | 97 | 57.264 | 53.257 | 5.624 | 1.00 | 12.02 | B_13 |
| ATOM | 2373 | CD2 | HIS | 97 | 57.214 | 53.603 | 6.929 | 1.00 | 10.00 | B_13 |
| ATOM | 2374 | ND1 | HIS | 97 | 56.516 | 52.104 | 5.499 | 1.00 | 12.91 | B_13 |
| ATOM | 2375 | CE1 | HIS | 97 | 56.038 | 51.770 | 6.688 | 1.00 | 10.00 | B_13 |
| ATOM | 2376 | NE2 | HIS | 97 | 56.445 | 52.664 | 7.571 | 1.00 | 10.64 | B_13 |
| ATOM | 2378 | C | HIS | 97 | 59.069 | 55.959 | 3.520 | 1.00 | 13.82 | B_13 |
| ATOM | 2379 | O | HIS | 97 | 58.415 | 56.273 | 2.517 | 1.00 | 12.27 | B_13 |
| ATOM | 2380 | N | PHE | 98 | 60.379 | 56.154 | 3.647 | 1.00 | 10.67 | B_13 |
| ATOM | 2382 | CA | PHE | 98 | 61.224 | 56.718 | 2.595 | 1.00 | 15.67 | B_13 |
| ATOM | 2383 | CB | PHE | 98 | 61.970 | 57.938 | 3.156 | 1.00 | 10.76 | B_13 |
| ATOM | 2384 | CG | PHE | 98 | 61.055 | 59.025 | 3.627 | 1.00 | 17.93 | B_13 |
| ATOM | 2385 | CD1 | PHE | 98 | 60.730 | 60.082 | 2.786 | 1.00 | 18.92 | B_13 |
| ATOM | 2386 | CD2 | PHE | 98 | 60.476 | 58.974 | 4.893 | 1.00 | 14.14 | B_13 |
| ATOM | 2387 | CE1 | PHE | 98 | 59.833 | 61.066 | 3.201 | 1.00 | 22.42 | B_13 |
| ATOM | 2388 | CE2 | PHE | 98 | 59.574 | 59.962 | 5.315 | 1.00 | 10.00 | B_13 |
| ATOM | 2389 | CZ | PHE | 98 | 59.257 | 61.002 | 4.469 | 1.00 | 10.00 | B_13 |
| ATOM | 2390 | C | PHE | 98 | 62.218 | 55.669 | 2.064 | 1.00 | 26.64 | B_13 |
| ATOM | 2391 | O | PHE | 98 | 62.882 | 54.969 | 2.851 | 1.00 | 13.27 | B_13 |
| ATOM | 2392 | N | ASP | 99 | 62.331 | 55.577 | 0.738 | 1.00 | 12.24 | B_13 |
| ATOM | 2394 | CA | ASP | 99 | 63.229 | 54.612 | 0.102 | 1.00 | 10.00 | B_13 |
| ATOM | 2395 | CB | ASP | 99 | 62.884 | 54.471 | -1.385 | 1.00 | 10.00 | B_13 |
| ATOM | 2396 | CG | ASP | 99 | 63.615 | 53.311 | -2.067 | 1.00 | 22.86 | B_13 |
| ATOM | 2397 | OD1 | ASP | 99 | 63.170 | 52.890 | -3.160 | 1.00 | 11.60 | B_13 |
| ATOM | 2398 | OD2 | ASP | 99 | 64.624 | 52.806 | -1.528 | 1.00 | 21.20 | B_13 |
| ATOM | 2399 | C | ASP | 99 | 64.677 | 55.046 | 0.264 | 1.00 | 12.66 | B_13 |
| ATOM | 2400 | O | ASP | 99 | 65.121 | 56.010 | -0.366 | 1.00 | 18.37 | B_13 |
| ATOM | 2401 | N | ASP | 100 | 65.439 | 54.289 | 1.046 | 1.00 | 12.86 | B_13 |
| ATOM | 2403 | CA | ASP | 100 | 66.833 | 54.642 | 1.260 | 1.00 | 14.46 | B_13 |
| ATOM | 2404 | CB | ASP | 100 | 67.308 | 54.271 | 2.660 | 1.00 | 17.70 | B_13 |
| ATOM | 2405 | CG | ASP | 100 | 68.006 | 55.437 | 3.358 | 1.00 | 16.15 | B_13 |
| ATOM | 2406 | OD1 | ASP | 100 | 68.091 | 55.447 | 4.602 | 1.00 | 15.74 | B_13 |
| ATOM | 2407 | OD2 | ASP | 100 | 68.470 | 56.354 | 2.655 | 1.00 | 27.08 | B_13 |
| ATOM | 2408 | C | ASP | 100 | 67.793 | 54.171 | 0.179 | 1.00 | 13.66 | B_13 |
| ATOM | 2409 | O | ASP | 100 | 68.961 | 53.932 | 0.416 | 1.00 | 19.54 | B_13 |
| ATOM | 2410 | N | ASP | 101 | 67.254 | 53.954 | -1.010 | 1.00 | 12.83 | B_13 |
| ATOM | 2412 | CA | ASP | 101 | 68.074 | 53.590 | -2.164 | 1.00 | 10.00 | B_13 |
| ATOM | 2413 | CB | ASP | 101 | 67.471 | 52.413 | -2.933 | 1.00 | 10.00 | B_13 |
| ATOM | 2414 | CG | ASP | 101 | 67.997 | 51.065 | -2.449 | 1.00 | 16.87 | B_13 |
| ATOM | 2415 | OD1 | ASP | 101 | 67.232 | 50.089 | -2.458 | 1.00 | 19.89 | B_13 |
| ATOM | 2416 | OD2 | ASP | 101 | 69.184 | 50.968 | -2.066 | 1.00 | 18.51 | B_13 |
| ATOM | 2417 | C | ASP | 101 | 68.108 | 54.858 | -3.029 | 1.00 | 26.72 | B_13 |
| ATOM | 2418 | O | ASP | 101 | 68.602 | 54.853 | -4.172 | 1.00 | 12.11 | B_13 |
| ATOM | 2419 | N | GLU | 102 | 67.500 | 55.922 | -2.496 | 1.00 | 13.76 | B_13 |
| ATOM | 2421 | CA | GLU | 102 | 67.462 | 57.217 | -3.161 | 1.00 | 12.54 | B_13 |
| ATOM | 2422 | CB | GLU | 102 | 66.135 | 57.958 | -2.916 | 1.00 | 13.01 | B_13 |
| ATOM | 2423 | CG | GLU | 102 | 64.873 | 57.257 | -3.381 | 1.00 | 15.50 | B_13 |
| ATOM | 2424 | CD | GLU | 102 | 64.973 | 56.707 | -4.791 | 1.00 | 29.02 | B_13 |
| ATOM | 2425 | OE1 | GLU | 102 | 65.640 | 57.307 | -5.665 | 1.00 | 12.78 | B_13 |
| ATOM | 2426 | OE2 | GLU | 102 | 64.399 | 55.635 | -5.021 | 1.00 | 12.36 | B_13 |
| ATOM | 2427 | C | GLU | 102 | 68.544 | 58.040 | -2.505 | 1.00 | 14.96 | B_13 |
| ATOM | 2428 | O | GLU | 102 | 68.939 | 57.760 | -1.371 | 1.00 | 10.00 | B_13 |
| ATOM | 2429 | N | THR | 103 | 69.030 | 59.039 | -3.228 | 1.00 | 19.38 | B_13 |
| ATOM | 2431 | CA | THR | 103 | 70.021 | 59.957 | -2.693 | 1.00 | 16.49 | B_13 |
| ATOM | 2432 | CB | THR | 103 | 70.973 | 60.490 | -3.801 | 1.00 | 19.31 | B_13 |
| ATOM | 2433 | OG1 | THR | 103 | 71.661 | 59.384 | -4.399 | 1.00 | 25.44 | B_13 |
| ATOM | 2435 | CG2 | THR | 103 | 72.006 | 61.462 | -3.212 | 1.00 | 10.75 | B_13 |
| ATOM | 2436 | C | THR | 103 | 69.180 | 61.104 | -2.141 | 1.00 | 12.91 | B_13 |
| ATOM | 2437 | O | THR | 103 | 68.414 | 61.727 | -2.867 | 1.00 | 13.59 | B_13 |
| ATOM | 2438 | N | TRP | 104 | 69.252 | 61.322 | -0.842 | 1.00 | 20.60 | B_13 |
| ATOM | 2440 | CA | TRP | 104 | 68.497 | 62.388 | -0.237 | 1.00 | 13.62 | B_13 |
| ATOM | 2441 | CB | TRP | 104 | 67.852 | 61.902 | 1.063 | 1.00 | 22.66 | B_13 |
| ATOM | 2442 | CG | TRP | 104 | 66.837 | 60.808 | 0.870 | 1.00 | 22.99 | B_13 |
| ATOM | 2443 | CD2 | TRP | 104 | 65.505 | 60.953 | 0.347 | 1.00 | 27.35 | B_13 |
| ATOM | 2444 | CE2 | TRP | 104 | 64.936 | 59.654 | 0.287 | 1.00 | 12.61 | B_13 |
| ATOM | 2445 | CE3 | TRP | 104 | 64.741 | 62.054 | -0.079 | 1.00 | 11.89 | B_13 |
| ATOM | 2446 | CD1 | TRP | 104 | 67.013 | 59.473 | 1.108 | 1.00 | 17.89 | B_13 |
| ATOM | 2447 | NE1 | TRP | 104 | 65.876 | 58.775 | 0.755 | 1.00 | 14.24 | B_13 |
| ATOM | 2449 | CZ2 | TRP | 104 | 63.632 | 59.429 | -0.186 | 1.00 | 10.00 | B_13 |
| ATOM | 2450 | CZ3 | TRP | 104 | 63.445 | 61.832 | -0.549 | 1.00 | 22.21 | B_13 |
| ATOM | 2451 | CH2 | TRP | 104 | 62.904 | 60.527 | -0.598 | 1.00 | 23.31 | B_13 |
| ATOM | 2452 | C | TRP | 104 | 69.416 | 63.570 | 0.033 | 1.00 | 16.43 | B_13 |

64/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2453 | O | TRP | 104 | 70.520 | 63.380 | 0.526 | 1.00 | 11.13 | B_13 |
| ATOM | 2454 | N | THR | 105 | 68.960 | 64.775 | -0.322 | 1.00 | 19.48 | B_13 |
| ATOM | 2456 | CA | THR | 105 | 69.716 | 66.015 | -0.097 | 1.00 | 10.40 | B_13 |
| ATOM | 2457 | CB | THR | 105 | 70.153 | 66.749 | -1.398 | 1.00 | 10.00 | B_13 |
| ATOM | 2458 | OG1 | THR | 105 | 69.305 | 66.401 | -2.501 | 1.00 | 18.53 | B_13 |
| ATOM | 2460 | CG2 | THR | 105 | 71.596 | 66.484 | -1.709 | 1.00 | 34.62 | B_13 |
| ATOM | 2461 | C | THR | 105 | 68.904 | 67.062 | 0.641 | 1.00 | 20.82 | B_13 |
| ATOM | 2462 | O | THR | 105 | 67.686 | 66.952 | 0.768 | 1.00 | 15.93 | B_13 |
| ATOM | 2463 | N | SER | 106 | 69.621 | 68.073 | 1.125 | 1.00 | 38.37 | B_13 |
| ATOM | 2465 | CA | SER | 106 | 69.029 | 69.222 | 1.791 | 1.00 | 20.77 | B_13 |
| ATOM | 2466 | CB | SER | 106 | 69.979 | 69.778 | 2.862 | 1.00 | 17.95 | B_13 |
| ATOM | 2467 | OG | SER | 106 | 70.281 | 68.825 | 3.864 | 1.00 | 29.88 | B_13 |
| ATOM | 2469 | C | SER | 106 | 68.889 | 70.245 | 0.657 | 1.00 | 19.23 | B_13 |
| ATOM | 2470 | O | SER | 106 | 68.202 | 71.260 | 0.782 | 1.00 | 21.34 | B_13 |
| ATOM | 2471 | N | SER | 107 | 69.577 | 69.981 | -0.450 | 1.00 | 18.73 | B_13 |
| ATOM | 2473 | CA | SER | 107 | 69.533 | 70.884 | -1.592 | 1.00 | 20.92 | B_13 |
| ATOM | 2474 | CB | SER | 107 | 70.945 | 71.380 | -1.927 | 1.00 | 19.84 | B_13 |
| ATOM | 2475 | OG | SER | 107 | 71.556 | 71.957 | -0.788 | 1.00 | 27.31 | B_13 |
| ATOM | 2477 | C | SER | 107 | 68.848 | 70.284 | -2.828 | 1.00 | 18.68 | B_13 |
| ATOM | 2478 | O | SER | 107 | 67.660 | 69.953 | -2.771 | 1.00 | 21.51 | B_13 |
| ATOM | 2479 | N | SER | 108 | 69.623 | 70.038 | -3.888 | 1.00 | 18.53 | B_13 |
| ATOM | 2481 | CA | SER | 108 | 69.091 | 69.544 | -5.152 | 1.00 | 16.21 | B_13 |
| ATOM | 2482 | CB | SER | 108 | 69.285 | 70.632 | -6.205 | 1.00 | 29.10 | B_13 |
| ATOM | 2483 | OG | SER | 108 | 70.665 | 70.969 | -6.271 | 1.00 | 21.47 | B_13 |
| ATOM | 2485 | C | SER | 108 | 69.645 | 68.260 | -5.745 | 1.00 | 17.68 | B_13 |
| ATOM | 2486 | O | SER | 108 | 68.964 | 67.618 | -6.541 | 1.00 | 19.67 | B_13 |
| ATOM | 2487 | N | LYS | 109 | 70.895 | 67.919 | -5.448 | 1.00 | 11.70 | B_13 |
| ATOM | 2489 | CA | LYS | 109 | 71.468 | 66.721 | -6.047 | 1.00 | 10.00 | B_13 |
| ATOM | 2490 | CB | LYS | 109 | 72.994 | 66.748 | -5.989 | 1.00 | 18.86 | B_13 |
| ATOM | 2491 | CG | LYS | 109 | 73.657 | 65.833 | -7.013 | 1.00 | 16.33 | B_13 |
| ATOM | 2492 | CD | LYS | 109 | 75.143 | 65.726 | -6.740 | 1.00 | 11.58 | B_13 |
| ATOM | 2493 | CE | LYS | 109 | 75.787 | 64.655 | -7.606 | 1.00 | 27.43 | B_13 |
| ATOM | 2494 | NZ | LYS | 109 | 77.218 | 64.492 | -7.251 | 1.00 | 35.03 | B_13 |
| ATOM | 2498 | C | LYS | 109 | 70.916 | 65.428 | -5.444 | 1.00 | 29.39 | B_13 |
| ATOM | 2499 | O | LYS | 109 | 71.432 | 64.905 | -4.449 | 1.00 | 29.95 | B_13 |
| ATOM | 2500 | N | GLY | 110 | 69.852 | 64.922 | -6.055 | 1.00 | 14.77 | B_13 |
| ATOM | 2502 | CA | GLY | 110 | 69.227 | 63.705 | -5.576 | 1.00 | 24.08 | B_13 |
| ATOM | 2503 | C | GLY | 110 | 67.793 | 64.105 | -5.342 | 1.00 | 20.25 | B_13 |
| ATOM | 2504 | O | GLY | 110 | 67.203 | 64.737 | -6.198 | 1.00 | 16.21 | B_13 |
| ATOM | 2505 | N | TYR | 111 | 67.248 | 63.772 | -4.182 | 1.00 | 10.00 | B_13 |
| ATOM | 2507 | CA | TYR | 111 | 65.879 | 64.130 | -3.845 | 1.00 | 24.52 | B_13 |
| ATOM | 2508 | CB | TYR | 111 | 65.030 | 62.868 | -3.688 | 1.00 | 22.46 | B_13 |
| ATOM | 2509 | CG | TYR | 111 | 64.676 | 62.244 | -4.999 | 1.00 | 10.83 | B_13 |
| ATOM | 2510 | CD1 | TYR | 111 | 65.380 | 61.155 | -5.483 | 1.00 | 25.38 | B_13 |
| ATOM | 2511 | CE1 | TYR | 111 | 65.068 | 60.592 | -6.720 | 1.00 | 18.68 | B_13 |
| ATOM | 2512 | CD2 | TYR | 111 | 63.646 | 62.769 | -5.776 | 1.00 | 16.02 | B_13 |
| ATOM | 2513 | CE2 | TYR | 111 | 63.328 | 62.223 | -7.013 | 1.00 | 31.72 | B_13 |
| ATOM | 2514 | CZ | TYR | 111 | 64.041 | 61.131 | -7.473 | 1.00 | 23.68 | B_13 |
| ATOM | 2515 | OH | TYR | 111 | 63.711 | 60.550 | -8.666 | 1.00 | 20.96 | B_13 |
| ATOM | 2517 | C | TYR | 111 | 65.856 | 64.944 | -2.553 | 1.00 | 22.83 | B_13 |
| ATOM | 2518 | O | TYR | 111 | 66.410 | 64.518 | -1.538 | 1.00 | 11.66 | B_13 |
| ATOM | 2519 | N | ASN | 112 | 65.278 | 66.140 | -2.611 | 1.00 | 17.47 | B_13 |
| ATOM | 2521 | CA | ASN | 112 | 65.180 | 67.006 | -1.431 | 1.00 | 15.77 | B_13 |
| ATOM | 2522 | CB | ASN | 112 | 64.658 | 68.401 | -1.817 | 1.00 | 15.93 | B_13 |
| ATOM | 2523 | CG | ASN | 112 | 64.694 | 69.384 | -0.657 | 1.00 | 10.00 | B_13 |
| ATOM | 2524 | OD1 | ASN | 112 | 63.757 | 69.465 | 0.132 | 1.00 | 15.33 | B_13 |
| ATOM | 2525 | ND2 | ASN | 112 | 65.754 | 70.180 | -0.586 | 1.00 | 13.70 | B_13 |
| ATOM | 2528 | C | ASN | 112 | 64.214 | 66.329 | -0.472 | 1.00 | 17.73 | B_13 |
| ATOM | 2529 | O | ASN | 112 | 63.007 | 66.243 | -0.737 | 1.00 | 12.61 | B_13 |
| ATOM | 2530 | N | LEU | 113 | 64.755 | 65.830 | 0.630 | 1.00 | 16.28 | B_13 |
| ATOM | 2532 | CA | LEU | 113 | 63.962 | 65.121 | 1.619 | 1.00 | 15.93 | B_13 |
| ATOM | 2533 | CB | LEU | 113 | 64.841 | 64.703 | 2.804 | 1.00 | 11.93 | B_13 |
| ATOM | 2534 | CG | LEU | 113 | 64.719 | 63.352 | 3.521 | 1.00 | 17.15 | B_13 |
| ATOM | 2535 | CD1 | LEU | 113 | 65.002 | 63.640 | 4.987 | 1.00 | 10.00 | B_13 |
| ATOM | 2536 | CD2 | LEU | 113 | 63.370 | 62.667 | 3.362 | 1.00 | 16.08 | B_13 |
| ATOM | 2537 | C | LEU | 113 | 62.802 | 65.994 | 2.085 | 1.00 | 14.61 | B_13 |
| ATOM | 2538 | O | LEU | 113 | 61.673 | 65.528 | 2.161 | 1.00 | 17.98 | B_13 |
| ATOM | 2539 | N | PHE | 114 | 63.073 | 67.267 | 2.346 | 1.00 | 16.81 | B_13 |
| ATOM | 2541 | CA | PHE | 114 | 62.056 | 68.212 | 2.791 | 1.00 | 15.65 | B_13 |
| ATOM | 2542 | CB | PHE | 114 | 62.638 | 69.630 | 2.888 | 1.00 | 22.16 | B_13 |
| ATOM | 2543 | CG | PHE | 114 | 61.596 | 70.714 | 2.882 | 1.00 | 12.27 | B_13 |
| ATOM | 2544 | CD1 | PHE | 114 | 60.804 | 70.952 | 4.004 | 1.00 | 19.93 | B_13 |
| ATOM | 2545 | CD2 | PHE | 114 | 61.378 | 71.470 | 1.746 | 1.00 | 13.56 | B_13 |
| ATOM | 2546 | CE1 | PHE | 114 | 59.813 | 71.932 | 3.984 | 1.00 | 17.08 | B_13 |
| ATOM | 2547 | CE2 | PHE | 114 | 60.398 | 72.441 | 1.726 | 1.00 | 13.79 | B_13 |
| ATOM | 2548 | CZ | PHE | 114 | 59.615 | 72.666 | 2.848 | 1.00 | 10.70 | B_13 |
| ATOM | 2549 | C | PHE | 114 | 60.860 | 68.220 | 1.842 | 1.00 | 19.55 | B_13 |

65/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2550 | O | PHE | 114 | 59.714 | 68.156 | 2.285 | 1.00 | 15.97 | B_13 |
| ATOM | 2551 | N | LEU | 115 | 61.135 | 68.309 | 0.543 | 1.00 | 13.35 | B_13 |
| ATOM | 2553 | CA | LEU | 115 | 60.096 | 68.323 | -0.485 | 1.00 | 17.91 | B_13 |
| ATOM | 2554 | CB | LEU | 115 | 60.741 | 68.462 | -1.868 | 1.00 | 24.65 | B_13 |
| ATOM | 2555 | CG | LEU | 115 | 60.501 | 69.739 | -2.679 | 1.00 | 22.70 | B_13 |
| ATOM | 2556 | CD1 | LEU | 115 | 61.033 | 70.939 | -1.943 | 1.00 | 17.98 | B_13 |
| ATOM | 2557 | CD2 | LEU | 115 | 61.148 | 69.624 | -4.048 | 1.00 | 28.50 | B_13 |
| ATOM | 2558 | C | LEU | 115 | 59.235 | 67.042 | -0.443 | 1.00 | 21.61 | B_13 |
| ATOM | 2559 | O | LEU | 115 | 58.002 | 67.093 | -0.344 | 1.00 | 13.99 | B_13 |
| ATOM | 2560 | N | VAL | 116 | 59.898 | 65.895 | -0.511 | 1.00 | 11.14 | B_13 |
| ATOM | 2562 | CA | VAL | 116 | 59.199 | 64.616 | -0.482 | 1.00 | 22.27 | B_13 |
| ATOM | 2563 | CB | VAL | 116 | 60.163 | 63.421 | -0.772 | 1.00 | 17.40 | B_13 |
| ATOM | 2564 | CG1 | VAL | 116 | 59.437 | 62.086 | -0.629 | 1.00 | 23.09 | B_13 |
| ATOM | 2565 | CG2 | VAL | 116 | 60.741 | 63.534 | -2.169 | 1.00 | 12.16 | B_13 |
| ATOM | 2566 | C | VAL | 116 | 58.502 | 64.414 | 0.864 | 1.00 | 10.00 | B_13 |
| ATOM | 2567 | O | VAL | 116 | 57.368 | 63.950 | 0.911 | 1.00 | 16.18 | B_13 |
| ATOM | 2568 | N | ALA | 117 | 59.153 | 64.803 | 1.954 | 1.00 | 10.00 | B_13 |
| ATOM | 2570 | CA | ALA | 117 | 58.585 | 64.640 | 3.297 | 1.00 | 19.50 | B_13 |
| ATOM | 2571 | CB | ALA | 117 | 59.608 | 64.995 | 4.352 | 1.00 | 11.81 | B_13 |
| ATOM | 2572 | C | ALA | 117 | 57.309 | 65.455 | 3.505 | 1.00 | 30.87 | B_13 |
| ATOM | 2573 | O | ALA | 117 | 56.327 | 64.955 | 4.053 | 1.00 | 10.00 | B_13 |
| ATOM | 2574 | N | ALA | 118 | 57.322 | 66.714 | 3.087 | 1.00 | 24.62 | B_13 |
| ATOM | 2576 | CA | ALA | 118 | 56.140 | 67.553 | 3.222 | 1.00 | 20.76 | B_13 |
| ATOM | 2577 | CB | ALA | 118 | 56.407 | 68.917 | 2.654 | 1.00 | 16.19 | B_13 |
| ATOM | 2578 | C | ALA | 118 | 54.968 | 66.894 | 2.485 | 1.00 | 20.54 | B_13 |
| ATOM | 2579 | O | ALA | 118 | 53.843 | 66.889 | 2.981 | 1.00 | 22.12 | B_13 |
| ATOM | 2580 | N | HIS | 119 | 55.255 | 66.315 | 1.321 | 1.00 | 10.00 | B_13 |
| ATOM | 2582 | CA | HIS | 119 | 54.259 | 65.647 | 0.489 | 1.00 | 17.27 | B_13 |
| ATOM | 2583 | CB | HIS | 119 | 54.909 | 65.263 | -0.860 | 1.00 | 11.16 | B_13 |
| ATOM | 2584 | CG | HIS | 119 | 54.006 | 64.530 | -1.813 | 1.00 | 26.59 | B_13 |
| ATOM | 2585 | CD2 | HIS | 119 | 53.377 | 63.335 | -1.706 | 1.00 | 16.63 | B_13 |
| ATOM | 2586 | ND1 | HIS | 119 | 53.723 | 64.995 | -3.085 | 1.00 | 12.44 | B_13 |
| ATOM | 2588 | CE1 | HIS | 119 | 52.961 | 64.124 | -3.715 | 1.00 | 14.58 | B_13 |
| ATOM | 2589 | NE2 | HIS | 119 | 52.734 | 63.101 | -2.901 | 1.00 | 26.44 | B_13 |
| ATOM | 2590 | C | HIS | 119 | 53.722 | 64.419 | 1.227 | 1.00 | 17.00 | B_13 |
| ATOM | 2591 | O | HIS | 119 | 52.510 | 64.218 | 1.331 | 1.00 | 17.01 | B_13 |
| ATOM | 2592 | N | GLU | 120 | 54.626 | 63.607 | 1.751 | 1.00 | 10.31 | B_13 |
| ATOM | 2594 | CA | GLU | 120 | 54.231 | 62.401 | 2.466 | 1.00 | 12.32 | B_13 |
| ATOM | 2595 | CB | GLU | 120 | 55.463 | 61.627 | 2.961 | 1.00 | 15.34 | B_13 |
| ATOM | 2596 | CG | GLU | 120 | 56.354 | 61.078 | 1.848 | 1.00 | 10.00 | B_13 |
| ATOM | 2597 | CD | GLU | 120 | 55.574 | 60.260 | 0.867 | 1.00 | 18.64 | B_13 |
| ATOM | 2598 | OE1 | GLU | 120 | 55.598 | 60.565 | -0.348 | 1.00 | 18.08 | B_13 |
| ATOM | 2599 | OE2 | GLU | 120 | 54.920 | 59.308 | 1.320 | 1.00 | 14.49 | B_13 |
| ATOM | 2600 | C | GLU | 120 | 53.347 | 62.777 | 3.635 | 1.00 | 12.41 | B_13 |
| ATOM | 2601 | O | GLU | 120 | 52.323 | 62.130 | 3.888 | 1.00 | 26.62 | B_13 |
| ATOM | 2602 | N | PHE | 121 | 53.750 | 63.813 | 4.359 | 1.00 | 10.29 | B_13 |
| ATOM | 2604 | CA | PHE | 121 | 52.993 | 64.286 | 5.506 | 1.00 | 14.37 | B_13 |
| ATOM | 2605 | CB | PHE | 121 | 53.780 | 65.344 | 6.270 | 1.00 | 20.10 | B_13 |
| ATOM | 2606 | CG | PHE | 121 | 55.057 | 64.827 | 6.852 | 1.00 | 24.55 | B_13 |
| ATOM | 2607 | CD1 | PHE | 121 | 56.037 | 65.700 | 7.292 | 1.00 | 10.00 | B_13 |
| ATOM | 2608 | CD2 | PHE | 121 | 55.292 | 63.454 | 6.936 | 1.00 | 23.62 | B_13 |
| ATOM | 2609 | CE1 | PHE | 121 | 57.247 | 65.212 | 7.813 | 1.00 | 18.59 | B_13 |
| ATOM | 2610 | CE2 | PHE | 121 | 56.488 | 62.954 | 7.448 | 1.00 | 15.21 | B_13 |
| ATOM | 2611 | CZ | PHE | 121 | 57.472 | 63.834 | 7.888 | 1.00 | 25.40 | B_13 |
| ATOM | 2612 | C | PHE | 121 | 51.607 | 64.791 | 5.110 | 1.00 | 16.63 | B_13 |
| ATOM | 2613 | O | PHE | 121 | 50.676 | 64.760 | 5.921 | 1.00 | 26.80 | B_13 |
| ATOM | 2614 | N | GLY | 122 | 51.471 | 65.238 | 3.864 | 1.00 | 11.98 | B_13 |
| ATOM | 2616 | CA | GLY | 122 | 50.175 | 65.664 | 3.380 | 1.00 | 12.95 | B_13 |
| ATOM | 2617 | C | GLY | 122 | 49.284 | 64.427 | 3.381 | 1.00 | 13.71 | B_13 |
| ATOM | 2618 | O | GLY | 122 | 48.113 | 64.483 | 3.753 | 1.00 | 13.74 | B_13 |
| ATOM | 2619 | N | HIS | 123 | 49.859 | 63.284 | 3.016 | 1.00 | 16.90 | B_13 |
| ATOM | 2621 | CA | HIS | 123 | 49.126 | 62.009 | 3.008 | 1.00 | 24.90 | B_13 |
| ATOM | 2622 | CB | HIS | 123 | 49.918 | 60.918 | 2.279 | 1.00 | 18.28 | B_13 |
| ATOM | 2623 | CG | HIS | 123 | 49.945 | 61.084 | 0.794 | 1.00 | 21.62 | B_13 |
| ATOM | 2624 | CD2 | HIS | 123 | 50.889 | 60.764 | -0.119 | 1.00 | 13.04 | B_13 |
| ATOM | 2625 | ND1 | HIS | 123 | 48.887 | 61.618 | 0.093 | 1.00 | 17.18 | B_13 |
| ATOM | 2627 | CE1 | HIS | 123 | 49.176 | 61.621 | -1.195 | 1.00 | 16.02 | B_13 |
| ATOM | 2628 | NE2 | HIS | 123 | 50.386 | 61.108 | -1.353 | 1.00 | 15.58 | B_13 |
| ATOM | 2629 | C | HIS | 123 | 48.864 | 61.562 | 4.446 | 1.00 | 19.74 | B_13 |
| ATOM | 2630 | O | HIS | 123 | 47.744 | 61.179 | 4.785 | 1.00 | 15.41 | B_13 |
| ATOM | 2631 | N | SER | 124 | 49.904 | 61.627 | 5.284 | 1.00 | 13.32 | B_13 |
| ATOM | 2633 | CA | SER | 124 | 49.813 | 61.270 | 6.695 | 1.00 | 27.50 | B_13 |
| ATOM | 2634 | CB | SER | 124 | 51.131 | 61.582 | 7.425 | 1.00 | 18.63 | B_13 |
| ATOM | 2635 | OG | SER | 124 | 52.221 | 60.837 | 6.925 | 1.00 | 13.32 | B_13 |
| ATOM | 2637 | C | SER | 124 | 48.703 | 62.102 | 7.335 | 1.00 | 13.76 | B_13 |
| ATOM | 2638 | O | SER | 124 | 48.061 | 61.677 | 8.306 | 1.00 | 20.65 | B_13 |
| ATOM | 2639 | N | LEU | 125 | 48.481 | 63.300 | 6.814 | 1.00 | 13.33 | B_13 |

66/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2641 | CA | LEU | 125 | 47.439 | 64.133 | 7.387 | 1.00 | 24.62 | B_13 |
| ATOM | 2642 | CB | LEU | 125 | 47.893 | 65.592 | 7.436 | 1.00 | 20.76 | B_13 |
| ATOM | 2643 | CG | LEU | 125 | 49.076 | 65.849 | 8.383 | 1.00 | 14.66 | B_13 |
| ATOM | 2644 | CD1 | LEU | 125 | 49.739 | 67.159 | 8.064 | 1.00 | 16.16 | B_13 |
| ATOM | 2645 | CD2 | LEU | 125 | 48.610 | 65.811 | 9.822 | 1.00 | 16.44 | B_13 |
| ATOM | 2646 | C | LEU | 125 | 46.058 | 63.966 | 6.724 | 1.00 | 24.77 | B_13 |
| ATOM | 2647 | O | LEU | 125 | 45.066 | 64.528 | 7.195 | 1.00 | 15.63 | B_13 |
| ATOM | 2648 | N | GLY | 126 | 45.988 | 63.192 | 5.644 | 1.00 | 17.38 | B_13 |
| ATOM | 2650 | CA | GLY | 126 | 44.700 | 62.968 | 5.001 | 1.00 | 22.41 | B_13 |
| ATOM | 2651 | C | GLY | 126 | 44.453 | 63.487 | 3.603 | 1.00 | 13.20 | B_13 |
| ATOM | 2652 | O | GLY | 126 | 43.349 | 63.366 | 3.096 | 1.00 | 20.86 | B_13 |
| ATOM | 2653 | N | LEU | 127 | 45.452 | 64.079 | 2.972 | 1.00 | 12.39 | B_13 |
| ATOM | 2655 | CA | LEU | 127 | 45.267 | 64.592 | 1.617 | 1.00 | 11.56 | B_13 |
| ATOM | 2656 | CB | LEU | 127 | 45.965 | 65.947 | 1.467 | 1.00 | 19.19 | B_13 |
| ATOM | 2657 | CG | LEU | 127 | 45.300 | 67.206 | 2.039 | 1.00 | 14.42 | B_13 |
| ATOM | 2658 | CD1 | LEU | 127 | 44.875 | 67.030 | 3.496 | 1.00 | 32.31 | B_13 |
| ATOM | 2659 | CD2 | LEU | 127 | 46.288 | 68.374 | 1.912 | 1.00 | 25.45 | B_13 |
| ATOM | 2660 | C | LEU | 127 | 45.770 | 63.619 | 0.550 | 1.00 | 26.54 | B_13 |
| ATOM | 2661 | O | LEU | 127 | 46.920 | 63.156 | 0.601 | 1.00 | 18.76 | B_13 |
| ATOM | 2662 | N | ASP | 128 | 44.908 | 63.285 | -0.407 | 1.00 | 28.54 | B_13 |
| ATOM | 2664 | CA | ASP | 128 | 45.292 | 62.376 | -1.480 | 1.00 | 10.89 | B_13 |
| ATOM | 2665 | CB | ASP | 128 | 44.059 | 61.762 | -2.136 | 1.00 | 15.95 | B_13 |
| ATOM | 2666 | CG | ASP | 128 | 44.351 | 60.430 | -2.794 | 1.00 | 23.44 | B_13 |
| ATOM | 2667 | OD1 | ASP | 128 | 43.377 | 59.735 | -3.164 | 1.00 | 41.43 | B_13 |
| ATOM | 2668 | OD2 | ASP | 128 | 45.541 | 60.059 | -2.918 | 1.00 | 18.12 | B_13 |
| ATOM | 2669 | C | ASP | 128 | 46.060 | 63.203 | -2.502 | 1.00 | 25.34 | B_13 |
| ATOM | 2670 | O | ASP | 128 | 46.489 | 64.308 | -2.213 | 1.00 | 16.36 | B_13 |
| ATOM | 2671 | N | HIS | 129 | 46.283 | 62.645 | -3.682 | 1.00 | 17.53 | B_13 |
| ATOM | 2673 | CA | HIS | 129 | 47.001 | 63.366 | -4.718 | 1.00 | 26.87 | B_13 |
| ATOM | 2674 | CB | HIS | 129 | 47.495 | 62.398 | -5.794 | 1.00 | 10.00 | B_13 |
| ATOM | 2675 | CG | HIS | 129 | 48.729 | 61.645 | -5.400 | 1.00 | 19.64 | B_13 |
| ATOM | 2676 | CD2 | HIS | 129 | 49.769 | 61.996 | -4.609 | 1.00 | 19.96 | B_13 |
| ATOM | 2677 | ND1 | HIS | 129 | 49.012 | 60.373 | -5.859 | 1.00 | 23.97 | B_13 |
| ATOM | 2679 | CE1 | HIS | 129 | 50.170 | 59.977 | -5.372 | 1.00 | 17.95 | B_13 |
| ATOM | 2680 | NE2 | HIS | 129 | 50.658 | 60.944 | -4.605 | 1.00 | 13.79 | B_13 |
| ATOM | 2681 | C | HIS | 129 | 46.153 | 64.457 | -5.360 | 1.00 | 39.97 | B_13 |
| ATOM | 2682 | O | HIS | 129 | 45.011 | 64.220 | -5.757 | 1.00 | 25.97 | B_13 |
| ATOM | 2683 | N | SER | 130 | 46.743 | 65.640 | -5.481 | 1.00 | 21.04 | B_13 |
| ATOM | 2685 | CA | SER | 130 | 46.090 | 66.776 | -6.109 | 1.00 | 16.72 | B_13 |
| ATOM | 2686 | CB | SER | 130 | 46.847 | 68.058 | -5.757 | 1.00 | 20.97 | B_13 |
| ATOM | 2687 | OG | SER | 130 | 46.358 | 69.154 | -6.502 | 1.00 | 25.52 | B_13 |
| ATOM | 2689 | C | SER | 130 | 46.098 | 66.582 | -7.622 | 1.00 | 24.66 | B_13 |
| ATOM | 2690 | O | SER | 130 | 46.779 | 65.694 | -8.145 | 1.00 | 29.24 | B_13 |
| ATOM | 2691 | N | LYS | 131 | 45.315 | 67.403 | -8.315 | 1.00 | 26.96 | B_13 |
| ATOM | 2693 | CA | LYS | 131 | 45.253 | 67.358 | -9.769 | 1.00 | 20.25 | B_13 |
| ATOM | 2694 | CB | LYS | 131 | 43.796 | 67.379 | -10.247 | 1.00 | 33.22 | B_13 |
| ATOM | 2695 | CG | LYS | 131 | 43.159 | 68.775 | -10.302 | 1.00 | 32.85 | B_13 |
| ATOM | 2696 | CD | LYS | 131 | 43.335 | 69.436 | -11.675 | 1.00 | 15.99 | B_13 |
| ATOM | 2697 | CE | LYS | 131 | 43.023 | 70.919 | -11.601 | 1.00 | 30.34 | B_13 |
| ATOM | 2698 | NZ | LYS | 131 | 43.879 | 71.647 | -10.600 | 1.00 | 30.44 | B_13 |
| ATOM | 2702 | C | LYS | 131 | 45.998 | 68.602 | -10.249 | 1.00 | 15.31 | B_13 |
| ATOM | 2703 | O | LYS | 131 | 46.414 | 68.698 | -11.402 | 1.00 | 30.72 | B_13 |
| ATOM | 2704 | N | ASP | 132 | 46.191 | 69.536 | -9.323 | 1.00 | 23.41 | B_13 |
| ATOM | 2706 | CA | ASP | 132 | 46.869 | 70.798 | -9.581 | 1.00 | 22.69 | B_13 |
| ATOM | 2707 | CB | ASP | 132 | 46.641 | 71.726 | -8.379 | 1.00 | 24.86 | B_13 |
| ATOM | 2708 | CG | ASP | 132 | 46.819 | 73.200 | -8.712 | 1.00 | 24.93 | B_13 |
| ATOM | 2709 | OD1 | ASP | 132 | 46.007 | 74.009 | -8.208 | 1.00 | 29.71 | B_13 |
| ATOM | 2710 | OD2 | ASP | 132 | 47.766 | 73.555 | -9.448 | 1.00 | 28.82 | B_13 |
| ATOM | 2711 | C | ASP | 132 | 48.358 | 70.497 | -9.728 | 1.00 | 14.97 | B_13 |
| ATOM | 2712 | O | ASP | 132 | 49.047 | 70.235 | -8.742 | 1.00 | 19.64 | B_13 |
| ATOM | 2713 | N | PRO | 133 | 48.874 | 70.538 | -10.964 | 1.00 | 16.94 | B_13 |
| ATOM | 2714 | CD | PRO | 133 | 48.209 | 70.971 | -12.199 | 1.00 | 21.42 | B_13 |
| ATOM | 2715 | CA | PRO | 133 | 50.293 | 70.264 | -11.215 | 1.00 | 19.34 | B_13 |
| ATOM | 2716 | CB | PRO | 133 | 50.457 | 70.636 | -12.690 | 1.00 | 20.48 | B_13 |
| ATOM | 2717 | CG | PRO | 133 | 49.347 | 71.636 | -12.929 | 1.00 | 21.80 | B_13 |
| ATOM | 2718 | C | PRO | 133 | 51.237 | 71.059 | -10.322 | 1.00 | 17.45 | B_13 |
| ATOM | 2719 | O | PRO | 133 | 52.319 | 70.590 | -10.006 | 1.00 | 23.30 | B_13 |
| ATOM | 2720 | N | GLY | 134 | 50.799 | 72.246 | -9.904 | 1.00 | 32.46 | B_13 |
| ATOM | 2722 | CA | GLY | 134 | 51.610 | 73.104 | -9.051 | 1.00 | 19.44 | B_13 |
| ATOM | 2723 | C | GLY | 134 | 51.306 | 72.958 | -7.569 | 1.00 | 22.33 | B_13 |
| ATOM | 2724 | O | GLY | 134 | 51.556 | 73.877 | -6.795 | 1.00 | 21.92 | B_13 |
| ATOM | 2725 | N | ALA | 135 | 50.698 | 71.836 | -7.190 | 1.00 | 34.71 | B_13 |
| ATOM | 2727 | CA | ALA | 135 | 50.355 | 71.580 | -5.794 | 1.00 | 18.35 | B_13 |
| ATOM | 2728 | CB | ALA | 135 | 48.948 | 70.987 | -5.690 | 1.00 | 14.30 | B_13 |
| ATOM | 2729 | C | ALA | 135 | 51.370 | 70.616 | -5.210 | 1.00 | 10.00 | B_13 |
| ATOM | 2730 | O | ALA | 135 | 51.739 | 69.647 | -5.858 | 1.00 | 17.52 | B_13 |
| ATOM | 2731 | N | LEU | 136 | 51.727 | 70.842 | -3.952 | 1.00 | 21.29 | B_13 |

67/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2733 | CA | LEU | 136 | 52.692 | 70.015 | -3.230 | 1.00 | 14.62 | B_13 |
| ATOM | 2734 | CB | LEU | 136 | 52.738 | 70.458 | -1.763 | 1.00 | 18.54 | B_13 |
| ATOM | 2735 | CG | LEU | 136 | 54.007 | 70.308 | -0.921 | 1.00 | 34.11 | B_13 |
| ATOM | 2736 | CD1 | LEU | 136 | 53.587 | 69.907 | 0.485 | 1.00 | 14.76 | B_13 |
| ATOM | 2737 | CD2 | LEU | 136 | 54.969 | 69.296 | -1.508 | 1.00 | 11.64 | B_13 |
| ATOM | 2738 | C | LEU | 136 | 52.232 | 68.564 | -3.287 | 1.00 | 13.50 | B_13 |
| ATOM | 2739 | O | LEU | 136 | 53.033 | 67.640 | -3.238 | 1.00 | 19.04 | B_13 |
| ATOM | 2740 | N | MET | 137 | 50.921 | 68.364 | -3.281 | 1.00 | 17.54 | B_13 |
| ATOM | 2742 | CA | MET | 137 | 50.360 | 67.019 | -3.324 | 1.00 | 25.11 | B_13 |
| ATOM | 2743 | CB | MET | 137 | 49.010 | 66.981 | -2.599 | 1.00 | 19.80 | B_13 |
| ATOM | 2744 | CG | MET | 137 | 49.083 | 67.312 | -1.117 | 1.00 | 15.35 | B_13 |
| ATOM | 2745 | SD | MET | 137 | 50.354 | 66.361 | -0.262 | 1.00 | 11.22 | B_13 |
| ATOM | 2746 | CE | MET | 137 | 49.882 | 64.680 | -0.764 | 1.00 | 13.90 | B_13 |
| ATOM | 2747 | C | MET | 137 | 50.254 | 66.387 | -4.721 | 1.00 | 28.08 | B_13 |
| ATOM | 2748 | O | MET | 137 | 49.730 | 65.268 | -4.863 | 1.00 | 12.18 | B_13 |
| ATOM | 2749 | N | PHE | 138 | 50.771 | 67.070 | -5.743 | 1.00 | 10.00 | B_13 |
| ATOM | 2751 | CA | PHE | 138 | 50.751 | 66.528 | -7.097 | 1.00 | 12.27 | B_13 |
| ATOM | 2752 | CB | PHE | 138 | 51.327 | 67.523 | -8.094 | 1.00 | 19.38 | B_13 |
| ATOM | 2753 | CG | PHE | 138 | 51.051 | 67.175 | -9.534 | 1.00 | 25.74 | B_13 |
| ATOM | 2754 | CD1 | PHE | 138 | 52.090 | 67.077 | -10.448 | 1.00 | 19.74 | B_13 |
| ATOM | 2755 | CD2 | PHE | 138 | 49.747 | 67.007 | -9.990 | 1.00 | 24.46 | B_13 |
| ATOM | 2756 | CE1 | PHE | 138 | 51.843 | 66.824 | -11.786 | 1.00 | 19.54 | B_13 |
| ATOM | 2757 | CE2 | PHE | 138 | 49.495 | 66.750 | -11.335 | 1.00 | 24.12 | B_13 |
| ATOM | 2758 | CZ | PHE | 138 | 50.544 | 66.664 | -12.230 | 1.00 | 18.15 | B_13 |
| ATOM | 2759 | C | PHE | 138 | 51.619 | 65.269 | -7.068 | 1.00 | 25.93 | B_13 |
| ATOM | 2760 | O | PHE | 138 | 52.658 | 65.226 | -6.414 | 1.00 | 12.50 | B_13 |
| ATOM | 2761 | N | PRO | 139 | 51.166 | 64.194 | -7.714 | 1.00 | 25.17 | B_13 |
| ATOM | 2762 | CD | PRO | 139 | 49.870 | 64.004 | -8.392 | 1.00 | 10.00 | B_13 |
| ATOM | 2763 | CA | PRO | 139 | 51.950 | 62.956 | -7.713 | 1.00 | 18.48 | B_13 |
| ATOM | 2764 | CB | PRO | 139 | 50.981 | 61.946 | -8.339 | 1.00 | 15.96 | B_13 |
| ATOM | 2765 | CG | PRO | 139 | 50.140 | 62.798 | -9.250 | 1.00 | 18.82 | B_13 |
| ATOM | 2766 | C | PRO | 139 | 53.299 | 62.950 | -8.430 | 1.00 | 17.22 | B_13 |
| ATOM | 2767 | O | PRO | 139 | 53.849 | 61.876 | -8.661 | 1.00 | 36.93 | B_13 |
| ATOM | 2768 | N | ILE | 140 | 53.844 | 64.114 | -8.767 | 1.00 | 24.48 | B_13 |
| ATOM | 2770 | CA | ILE | 140 | 55.118 | 64.155 | -9.477 | 1.00 | 20.03 | B_13 |
| ATOM | 2771 | CB | ILE | 140 | 54.996 | 64.807 | -10.892 | 1.00 | 18.71 | B_13 |
| ATOM | 2772 | CG2 | ILE | 140 | 56.334 | 64.709 | -11.639 | 1.00 | 23.96 | B_13 |
| ATOM | 2773 | CG1 | ILE | 140 | 53.932 | 64.113 | -11.724 | 1.00 | 24.68 | B_13 |
| ATOM | 2774 | CD1 | ILE | 140 | 53.861 | 64.669 | -13.125 | 1.00 | 25.83 | B_13 |
| ATOM | 2775 | C | ILE | 140 | 56.109 | 64.992 | -8.700 | 1.00 | 27.87 | B_13 |
| ATOM | 2776 | O | ILE | 140 | 55.758 | 66.043 | -8.248 | 1.00 | 22.39 | B_13 |
| ATOM | 2777 | N | TYR | 141 | 57.332 | 64.512 | -8.535 | 1.00 | 12.36 | B_13 |
| ATOM | 2779 | CA | TYR | 141 | 58.350 | 65.281 | -7.834 | 1.00 | 21.85 | B_13 |
| ATOM | 2780 | CB | TYR | 141 | 59.418 | 64.353 | -7.266 | 1.00 | 15.16 | B_13 |
| ATOM | 2781 | CG | TYR | 141 | 60.592 | 65.096 | -6.672 | 1.00 | 15.65 | B_13 |
| ATOM | 2782 | CD1 | TYR | 141 | 61.755 | 65.306 | -7.407 | 1.00 | 18.56 | B_13 |
| ATOM | 2783 | CE1 | TYR | 141 | 62.836 | 65.967 | -6.859 | 1.00 | 10.00 | B_13 |
| ATOM | 2784 | CD2 | TYR | 141 | 60.546 | 65.576 | -5.366 | 1.00 | 11.42 | B_13 |
| ATOM | 2785 | CE2 | TYR | 141 | 61.626 | 66.236 | -4.814 | 1.00 | 13.45 | B_13 |
| ATOM | 2786 | CZ | TYR | 141 | 62.770 | 66.429 | -5.567 | 1.00 | 10.00 | B_13 |
| ATOM | 2787 | OH | TYR | 141 | 63.841 | 67.109 | -5.016 | 1.00 | 18.97 | B_13 |
| ATOM | 2789 | C | TYR | 141 | 59.042 | 66.270 | -8.776 | 1.00 | 19.52 | B_13 |
| ATOM | 2790 | O | TYR | 141 | 59.709 | 65.859 | -9.727 | 1.00 | 21.37 | B_13 |
| ATOM | 2791 | N | THR | 142 | 58.932 | 67.556 | -8.465 | 1.00 | 23.99 | B_13 |
| ATOM | 2793 | CA | THR | 142 | 59.573 | 68.616 | -9.238 | 1.00 | 19.53 | B_13 |
| ATOM | 2794 | CB | THR | 142 | 58.515 | 69.578 | -9.807 | 1.00 | 10.00 | B_13 |
| ATOM | 2795 | OG1 | THR | 142 | 57.704 | 68.880 | -10.756 | 1.00 | 37.02 | B_13 |
| ATOM | 2797 | CG2 | THR | 142 | 59.151 | 70.757 | -10.457 | 1.00 | 34.35 | B_13 |
| ATOM | 2798 | C | THR | 142 | 60.483 | 69.332 | -8.235 | 1.00 | 19.89 | B_13 |
| ATOM | 2799 | O | THR | 142 | 60.120 | 69.513 | -7.076 | 1.00 | 25.67 | B_13 |
| ATOM | 2800 | N | TYR | 143 | 61.699 | 69.677 | -8.643 | 1.00 | 30.64 | B_13 |
| ATOM | 2802 | CA | TYR | 143 | 62.609 | 70.344 | -7.707 | 1.00 | 32.54 | B_13 |
| ATOM | 2803 | CB | TYR | 143 | 64.091 | 70.190 | -8.108 | 1.00 | 26.34 | B_13 |
| ATOM | 2804 | CG | TYR | 143 | 65.008 | 71.048 | -7.244 | 1.00 | 10.69 | B_13 |
| ATOM | 2805 | CD1 | TYR | 143 | 65.066 | 70.866 | -5.852 | 1.00 | 16.37 | B_13 |
| ATOM | 2806 | CE1 | TYR | 143 | 65.801 | 71.738 | -5.035 | 1.00 | 26.03 | B_13 |
| ATOM | 2807 | CD2 | TYR | 143 | 65.714 | 72.114 | -7.795 | 1.00 | 17.36 | B_13 |
| ATOM | 2808 | CE2 | TYR | 143 | 66.451 | 73.006 | -6.981 | 1.00 | 15.32 | B_13 |
| ATOM | 2809 | CZ | TYR | 143 | 66.489 | 72.810 | -5.610 | 1.00 | 10.00 | B_13 |
| ATOM | 2810 | OH | TYR | 143 | 67.184 | 73.665 | -4.790 | 1.00 | 27.84 | B_13 |
| ATOM | 2812 | C | TYR | 143 | 62.330 | 71.815 | -7.456 | 1.00 | 24.77 | B_13 |
| ATOM | 2813 | O | TYR | 143 | 62.201 | 72.611 | -8.399 | 1.00 | 26.19 | B_13 |
| ATOM | 2814 | N | THR | 144 | 62.292 | 72.160 | -6.170 | 1.00 | 22.23 | B_13 |
| ATOM | 2816 | CA | THR | 144 | 62.103 | 73.533 | -5.727 | 1.00 | 33.68 | B_13 |
| ATOM | 2817 | CB | THR | 144 | 60.668 | 73.814 | -5.189 | 1.00 | 28.06 | B_13 |
| ATOM | 2818 | OG1 | THR | 144 | 60.277 | 72.812 | -4.241 | 1.00 | 38.14 | B_13 |
| ATOM | 2820 | CG2 | THR | 144 | 59.681 | 73.857 | -6.346 | 1.00 | 48.73 | B_13 |

68/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2821 | C | THR | 144 | 63.178 | 73.893 | -4.695 | 1.00 | 35.52 | B_13 |
| ATOM | 2822 | O | THR | 144 | 64.207 | 74.465 | -5.064 | 1.00 | 39.57 | B_13 |
| ATOM | 2823 | N | GLY | 145 | 62.967 | 73.552 | -3.422 | 1.00 | 35.95 | B_13 |
| ATOM | 2825 | CA | GLY | 145 | 63.967 | 73.872 | -2.407 | 1.00 | 35.01 | B_13 |
| ATOM | 2826 | C | GLY | 145 | 63.509 | 74.025 | -0.965 | 1.00 | 26.81 | B_13 |
| ATOM | 2827 | O | GLY | 145 | 62.566 | 74.773 | -0.670 | 1.00 | 40.81 | B_13 |
| ATOM | 2828 | N | LYS | 146 | 64.302 | 73.439 | -0.066 | 1.00 | 27.13 | B_13 |
| ATOM | 2830 | CA | LYS | 146 | 64.071 | 73.423 | 1.389 | 1.00 | 23.89 | B_13 |
| ATOM | 2831 | CB | LYS | 146 | 65.163 | 72.548 | 2.049 | 1.00 | 29.08 | B_13 |
| ATOM | 2832 | CG | LYS | 146 | 64.992 | 72.209 | 3.524 | 1.00 | 19.99 | B_13 |
| ATOM | 2833 | CD | LYS | 146 | 66.079 | 71.224 | 3.913 | 1.00 | 20.44 | B_13 |
| ATOM | 2834 | CE | LYS | 146 | 66.181 | 71.010 | 5.402 | 1.00 | 24.16 | B_13 |
| ATOM | 2835 | NZ | LYS | 146 | 67.250 | 69.987 | 5.727 | 1.00 | 23.37 | B_13 |
| ATOM | 2839 | C | LYS | 146 | 63.926 | 74.778 | 2.124 | 1.00 | 18.98 | B_13 |
| ATOM | 2840 | O | LYS | 146 | 63.900 | 74.831 | 3.353 | 1.00 | 28.15 | B_13 |
| ATOM | 2841 | N | SER | 147 | 63.826 | 75.871 | 1.382 | 1.00 | 35.50 | B_13 |
| ATOM | 2843 | CA | SER | 147 | 63.661 | 77.185 | 1.992 | 1.00 | 31.59 | B_13 |
| ATOM | 2844 | CB | SER | 147 | 64.988 | 77.673 | 2.594 | 1.00 | 27.05 | B_13 |
| ATOM | 2845 | OG | SER | 147 | 65.996 | 77.756 | 1.586 | 1.00 | 48.28 | B_13 |
| ATOM | 2847 | C | SER | 147 | 63.203 | 78.131 | 0.902 | 1.00 | 27.12 | B_13 |
| ATOM | 2848 | O | SER | 147 | 62.743 | 79.251 | 1.168 | 1.00 | 33.75 | B_13 |
| ATOM | 2849 | N | HIS | 148 | 63.248 | 77.644 | -0.332 | 1.00 | 25.13 | B_13 |
| ATOM | 2851 | CA | HIS | 148 | 62.872 | 78.465 | -1.463 | 1.00 | 23.42 | B_13 |
| ATOM | 2852 | CB | HIS | 148 | 63.704 | 78.076 | -2.678 | 1.00 | 17.40 | B_13 |
| ATOM | 2853 | CG | HIS | 148 | 65.174 | 78.020 | -2.398 | 1.00 | 45.97 | B_13 |
| ATOM | 2854 | CD2 | HIS | 148 | 66.204 | 77.524 | -3.121 | 1.00 | 27.24 | B_13 |
| ATOM | 2855 | ND1 | HIS | 148 | 65.724 | 78.476 | -1.213 | 1.00 | 43.49 | B_13 |
| ATOM | 2857 | CE1 | HIS | 148 | 67.024 | 78.253 | -1.218 | 1.00 | 30.28 | B_13 |
| ATOM | 2858 | NE2 | HIS | 148 | 67.342 | 77.676 | -2.366 | 1.00 | 45.28 | B_13 |
| ATOM | 2860 | C | HIS | 148 | 61.381 | 78.433 | -1.796 | 1.00 | 47.15 | B_13 |
| ATOM | 2861 | O | HIS | 148 | 60.936 | 79.166 | -2.704 | 1.00 | 40.97 | B_13 |
| ATOM | 2862 | N | PHE | 149 | 60.601 | 77.636 | -1.053 | 1.00 | 48.76 | B_13 |
| ATOM | 2864 | CA | PHE | 149 | 59.170 | 77.557 | -1.347 | 1.00 | 32.44 | B_13 |
| ATOM | 2865 | CB | PHE | 149 | 58.856 | 76.364 | -2.269 | 1.00 | 27.77 | B_13 |
| ATOM | 2866 | CG | PHE | 149 | 58.415 | 76.781 | -3.657 | 1.00 | 24.63 | B_13 |
| ATOM | 2867 | CD1 | PHE | 149 | 57.826 | 75.874 | -4.520 | 1.00 | 25.66 | B_13 |
| ATOM | 2868 | CD2 | PHE | 149 | 58.550 | 78.106 | -4.072 | 1.00 | 30.89 | B_13 |
| ATOM | 2869 | CE1 | PHE | 149 | 57.376 | 76.277 | -5.767 | 1.00 | 17.10 | B_13 |
| ATOM | 2870 | CE2 | PHE | 149 | 58.104 | 78.520 | -5.311 | 1.00 | 18.57 | B_13 |
| ATOM | 2871 | CZ | PHE | 149 | 57.513 | 77.608 | -6.166 | 1.00 | 30.20 | B_13 |
| ATOM | 2872 | C | PHE | 149 | 58.061 | 77.791 | -0.308 | 1.00 | 27.40 | B_13 |
| ATOM | 2873 | O | PHE | 149 | 58.299 | 77.971 | 0.892 | 1.00 | 29.69 | B_13 |
| ATOM | 2874 | N | MET | 150 | 56.836 | 77.729 | -0.822 | 1.00 | 28.66 | B_13 |
| ATOM | 2876 | CA | MET | 150 | 55.621 | 78.027 | -0.094 | 1.00 | 20.63 | B_13 |
| ATOM | 2877 | CB | MET | 150 | 55.251 | 79.431 | -0.503 | 1.00 | 25.60 | B_13 |
| ATOM | 2878 | CG | MET | 150 | 55.599 | 79.691 | -1.989 | 1.00 | 23.95 | B_13 |
| ATOM | 2879 | SD | MET | 150 | 57.336 | 80.086 | -2.296 | 1.00 | 76.68 | B_13 |
| ATOM | 2880 | CE | MET | 150 | 57.209 | 81.473 | -3.385 | 1.00 | 21.07 | B_13 |
| ATOM | 2881 | C | MET | 150 | 54.436 | 77.118 | -0.450 | 1.00 | 30.58 | B_13 |
| ATOM | 2882 | O | MET | 150 | 54.104 | 76.948 | -1.628 | 1.00 | 16.91 | B_13 |
| ATOM | 2883 | N | LEU | 151 | 53.727 | 76.664 | 0.581 | 1.00 | 36.94 | B_13 |
| ATOM | 2885 | CA | LEU | 151 | 52.576 | 75.772 | 0.431 | 1.00 | 25.68 | B_13 |
| ATOM | 2886 | CB | LEU | 151 | 51.968 | 75.474 | 1.807 | 1.00 | 23.46 | B_13 |
| ATOM | 2887 | CG | LEU | 151 | 51.087 | 74.232 | 1.927 | 1.00 | 24.21 | B_13 |
| ATOM | 2888 | CD1 | LEU | 151 | 51.936 | 72.998 | 1.657 | 1.00 | 21.54 | B_13 |
| ATOM | 2889 | CD2 | LEU | 151 | 50.487 | 74.150 | 3.314 | 1.00 | 19.89 | B_13 |
| ATOM | 2890 | C | LEU | 151 | 51.498 | 76.322 | -0.491 | 1.00 | 17.09 | B_13 |
| ATOM | 2891 | O | LEU | 151 | 50.795 | 77.267 | -0.136 | 1.00 | 35.38 | B_13 |
| ATOM | 2892 | N | PRO | 152 | 51.338 | 75.727 | -1.686 | 1.00 | 16.90 | B_13 |
| ATOM | 2893 | CD | PRO | 152 | 52.154 | 74.643 | -2.255 | 1.00 | 25.80 | B_13 |
| ATOM | 2894 | CA | PRO | 152 | 50.334 | 76.170 | -2.653 | 1.00 | 29.65 | B_13 |
| ATOM | 2895 | CB | PRO | 152 | 50.447 | 75.110 | -3.749 | 1.00 | 24.68 | B_13 |
| ATOM | 2896 | CG | PRO | 152 | 51.892 | 74.791 | -3.722 | 1.00 | 14.34 | B_13 |
| ATOM | 2897 | C | PRO | 152 | 48.910 | 76.261 | -2.087 | 1.00 | 10.00 | B_13 |
| ATOM | 2898 | O | PRO | 152 | 48.543 | 75.505 | -1.184 | 1.00 | 20.25 | B_13 |
| ATOM | 2899 | N | ASP | 153 | 48.117 | 77.180 | -2.639 | 1.00 | 19.53 | B_13 |
| ATOM | 2901 | CA | ASP | 153 | 46.723 | 77.387 | -2.226 | 1.00 | 15.90 | B_13 |
| ATOM | 2902 | CB | ASP | 153 | 45.986 | 78.304 | -3.213 | 1.00 | 22.34 | B_13 |
| ATOM | 2903 | CG | ASP | 153 | 46.418 | 79.741 | -3.115 | 1.00 | 28.86 | B_13 |
| ATOM | 2904 | OD1 | ASP | 153 | 47.016 | 80.115 | -2.074 | 1.00 | 35.34 | B_13 |
| ATOM | 2905 | OD2 | ASP | 153 | 46.142 | 80.494 | -4.084 | 1.00 | 30.09 | B_13 |
| ATOM | 2906 | C | ASP | 153 | 45.953 | 76.084 | -2.169 | 1.00 | 27.31 | B_13 |
| ATOM | 2907 | O | ASP | 153 | 45.309 | 75.783 | -1.167 | 1.00 | 23.50 | B_13 |
| ATOM | 2908 | N | ASP | 154 | 46.000 | 75.339 | -3.276 | 1.00 | 25.51 | B_13 |
| ATOM | 2910 | CA | ASP | 154 | 45.316 | 74.063 | -3.392 | 1.00 | 20.91 | B_13 |
| ATOM | 2911 | CB | ASP | 154 | 45.745 | 73.364 | -4.682 | 1.00 | 14.23 | B_13 |
| ATOM | 2912 | CG | ASP | 154 | 45.033 | 72.062 | -4.885 | 1.00 | 22.95 | B_13 |

69/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2913 | OD1 | ASP | 154 | 45.590 | 71.026 | -4.516 | 1.00 | 17.80 | B_13 |
| ATOM | 2914 | OD2 | ASP | 154 | 43.904 | 72.076 | -5.388 | 1.00 | 19.14 | B_13 |
| ATOM | 2915 | C | ASP | 154 | 45.551 | 73.155 | -2.173 | 1.00 | 26.95 | B_13 |
| ATOM | 2916 | O | ASP | 154 | 44.629 | 72.491 | -1.696 | 1.00 | 22.92 | B_13 |
| ATOM | 2917 | N | ASP | 155 | 46.776 | 73.155 | -1.654 | 1.00 | 23.56 | B_13 |
| ATOM | 2919 | CA | ASP | 155 | 47.110 | 72.338 | -0.490 | 1.00 | 28.69 | B_13 |
| ATOM | 2920 | CB | ASP | 155 | 48.618 | 72.118 | -0.388 | 1.00 | 12.87 | B_13 |
| ATOM | 2921 | CG | ASP | 155 | 49.208 | 71.566 | -1.676 | 1.00 | 24.35 | B_13 |
| ATOM | 2922 | OD1 | ASP | 155 | 49.705 | 72.369 | -2.500 | 1.00 | 27.89 | B_13 |
| ATOM | 2923 | OD2 | ASP | 155 | 49.152 | 70.335 | -1.875 | 1.00 | 16.96 | B_13 |
| ATOM | 2924 | C | ASP | 155 | 46.582 | 72.976 | 0.781 | 1.00 | 25.41 | B_13 |
| ATOM | 2925 | O | ASP | 155 | 46.055 | 72.275 | 1.656 | 1.00 | 13.36 | B_13 |
| ATOM | 2926 | N | VAL | 156 | 46.733 | 74.296 | 0.891 | 1.00 | 16.99 | B_13 |
| ATOM | 2928 | CA | VAL | 156 | 46.222 | 75.021 | 2.053 | 1.00 | 22.26 | B_13 |
| ATOM | 2929 | CB | VAL | 156 | 46.340 | 76.571 | 1.901 | 1.00 | 25.69 | B_13 |
| ATOM | 2930 | CG1 | VAL | 156 | 45.811 | 77.249 | 3.158 | 1.00 | 14.95 | B_13 |
| ATOM | 2931 | CG2 | VAL | 156 | 47.768 | 77.007 | 1.641 | 1.00 | 17.52 | B_13 |
| ATOM | 2932 | C | VAL | 156 | 44.727 | 74.705 | 2.129 | 1.00 | 10.00 | B_13 |
| ATOM | 2933 | O | VAL | 156 | 44.224 | 74.234 | 3.145 | 1.00 | 22.47 | B_13 |
| ATOM | 2934 | N | GLN | 157 | 44.033 | 74.980 | 1.029 | 1.00 | 16.19 | B_13 |
| ATOM | 2936 | CA | GLN | 157 | 42.604 | 74.758 | 0.930 | 1.00 | 17.97 | B_13 |
| ATOM | 2937 | CB | GLN | 157 | 42.108 | 75.039 | -0.497 | 1.00 | 17.10 | B_13 |
| ATOM | 2938 | CG | GLN | 157 | 40.804 | 75.852 | -0.547 | 1.00 | 26.00 | B_13 |
| ATOM | 2939 | CD | GLN | 157 | 40.949 | 77.284 | -0.005 | 1.00 | 25.84 | B_13 |
| ATOM | 2940 | OE1 | GLN | 157 | 41.218 | 77.505 | 1.177 | 1.00 | 39.61 | B_13 |
| ATOM | 2941 | NE2 | GLN | 157 | 40.744 | 78.255 | -0.875 | 1.00 | 32.22 | B_13 |
| ATOM | 2944 | C | GLN | 157 | 42.347 | 73.324 | 1.309 | 1.00 | 18.69 | B_13 |
| ATOM | 2945 | O | GLN | 157 | 41.368 | 73.015 | 1.982 | 1.00 | 10.00 | B_13 |
| ATOM | 2946 | N | GLY | 158 | 43.272 | 72.460 | 0.903 | 1.00 | 31.05 | B_13 |
| ATOM | 2948 | CA | GLY | 158 | 43.156 | 71.053 | 1.205 | 1.00 | 21.69 | B_13 |
| ATOM | 2949 | C | GLY | 158 | 43.129 | 70.738 | 2.684 | 1.00 | 13.51 | B_13 |
| ATOM | 2950 | O | GLY | 158 | 42.108 | 70.263 | 3.182 | 1.00 | 14.91 | B_13 |
| ATOM | 2951 | N | ILE | 159 | 44.224 | 71.006 | 3.398 | 1.00 | 19.34 | B_13 |
| ATOM | 2953 | CA | ILE | 159 | 44.268 | 70.686 | 4.827 | 1.00 | 19.14 | B_13 |
| ATOM | 2954 | CB | ILE | 159 | 45.669 | 70.880 | 5.503 | 1.00 | 12.57 | B_13 |
| ATOM | 2955 | CG2 | ILE | 159 | 46.268 | 69.542 | 5.960 | 1.00 | 19.22 | B_13 |
| ATOM | 2956 | CG1 | ILE | 159 | 46.603 | 71.702 | 4.633 | 1.00 | 31.62 | B_13 |
| ATOM | 2957 | CD1 | ILE | 159 | 46.426 | 73.177 | 4.824 | 1.00 | 25.87 | B_13 |
| ATOM | 2958 | C | ILE | 159 | 43.235 | 71.461 | 5.610 | 1.00 | 21.87 | B_13 |
| ATOM | 2959 | O | ILE | 159 | 42.691 | 70.952 | 6.592 | 1.00 | 21.02 | B_13 |
| ATOM | 2960 | N | GLN | 160 | 42.959 | 72.689 | 5.186 | 1.00 | 12.08 | B_13 |
| ATOM | 2962 | CA | GLN | 160 | 41.967 | 73.483 | 5.874 | 1.00 | 11.43 | B_13 |
| ATOM | 2963 | CB | GLN | 160 | 41.949 | 74.916 | 5.346 | 1.00 | 29.25 | B_13 |
| ATOM | 2964 | CG | GLN | 160 | 43.158 | 75.737 | 5.827 | 1.00 | 22.01 | B_13 |
| ATOM | 2965 | CD | GLN | 160 | 43.098 | 77.199 | 5.416 | 1.00 | 18.77 | B_13 |
| ATOM | 2966 | OE1 | GLN | 160 | 42.260 | 77.593 | 4.607 | 1.00 | 36.02 | B_13 |
| ATOM | 2967 | NE2 | GLN | 160 | 43.997 | 78.004 | 5.965 | 1.00 | 28.49 | B_13 |
| ATOM | 2970 | C | GLN | 160 | 40.596 | 72.820 | 5.772 | 1.00 | 22.28 | B_13 |
| ATOM | 2971 | O | GLN | 160 | 39.855 | 72.786 | 6.754 | 1.00 | 14.16 | B_13 |
| ATOM | 2972 | N | SER | 161 | 40.304 | 72.183 | 4.634 | 1.00 | 32.89 | B_13 |
| ATOM | 2974 | CA | SER | 161 | 39.005 | 71.537 | 4.474 | 1.00 | 29.25 | B_13 |
| ATOM | 2975 | CB | SER | 161 | 38.847 | 70.901 | 3.085 | 1.00 | 19.70 | B_13 |
| ATOM | 2976 | OG | SER | 161 | 39.594 | 69.706 | 2.946 | 1.00 | 24.88 | B_13 |
| ATOM | 2978 | C | SER | 161 | 38.831 | 70.503 | 5.566 | 1.00 | 22.08 | B_13 |
| ATOM | 2979 | O | SER | 161 | 37.745 | 70.340 | 6.118 | 1.00 | 26.26 | B_13 |
| ATOM | 2980 | N | LEU | 162 | 39.931 | 69.852 | 5.919 | 1.00 | 19.14 | B_13 |
| ATOM | 2982 | CA | LEU | 162 | 39.913 | 68.829 | 6.953 | 1.00 | 29.17 | B_13 |
| ATOM | 2983 | CB | LEU | 162 | 41.081 | 67.852 | 6.767 | 1.00 | 12.08 | B_13 |
| ATOM | 2984 | CG | LEU | 162 | 40.982 | 66.666 | 5.812 | 1.00 | 20.09 | B_13 |
| ATOM | 2985 | CD1 | LEU | 162 | 40.661 | 67.184 | 4.478 | 1.00 | 24.51 | B_13 |
| ATOM | 2986 | CD2 | LEU | 162 | 42.299 | 65.884 | 5.794 | 1.00 | 27.00 | B_13 |
| ATOM | 2987 | C | LEU | 162 | 39.965 | 69.392 | 8.364 | 1.00 | 24.75 | B_13 |
| ATOM | 2988 | O | LEU | 162 | 39.047 | 69.191 | 9.162 | 1.00 | 22.04 | B_13 |
| ATOM | 2989 | N | TYR | 163 | 41.015 | 70.151 | 8.652 | 1.00 | 20.72 | B_13 |
| ATOM | 2991 | CA | TYR | 163 | 41.211 | 70.689 | 9.980 | 1.00 | 10.00 | B_13 |
| ATOM | 2992 | CB | TYR | 163 | 42.695 | 70.595 | 10.343 | 1.00 | 10.95 | B_13 |
| ATOM | 2993 | CG | TYR | 163 | 43.221 | 69.167 | 10.209 | 1.00 | 10.00 | B_13 |
| ATOM | 2994 | CD1 | TYR | 163 | 43.114 | 68.261 | 11.264 | 1.00 | 37.53 | B_13 |
| ATOM | 2995 | CE1 | TYR | 163 | 43.452 | 66.913 | 11.103 | 1.00 | 26.00 | B_13 |
| ATOM | 2996 | CD2 | TYR | 163 | 43.703 | 68.689 | 8.990 | 1.00 | 23.78 | B_13 |
| ATOM | 2997 | CE2 | TYR | 163 | 44.048 | 67.342 | 8.822 | 1.00 | 17.88 | B_13 |
| ATOM | 2998 | CZ | TYR | 163 | 43.914 | 66.461 | 9.879 | 1.00 | 24.28 | B_13 |
| ATOM | 2999 | OH | TYR | 163 | 44.210 | 65.121 | 9.711 | 1.00 | 13.27 | B_13 |
| ATOM | 3001 | C | TYR | 163 | 40.634 | 72.085 | 10.187 | 1.00 | 26.45 | B_13 |
| ATOM | 3002 | O | TYR | 163 | 39.975 | 72.327 | 11.190 | 1.00 | 31.25 | B_13 |
| ATOM | 3003 | N | GLY | 164 | 40.819 | 72.975 | 9.219 | 1.00 | 29.43 | B_13 |
| ATOM | 3005 | CA | GLY | 164 | 40.291 | 74.324 | 9.340 | 1.00 | 30.64 | B_13 |

70/75

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 3006 | C | GLY | 164 | 41.402 | 75.344 | 9.424 | 1.00 | 30.89 | B_13 |
| ATOM | 3007 | O | GLY | 164 | 41.101 | 76.564 | 9.368 | 1.00 | 26.89 | B_13 |
| ATOM | 3008 | OT | GLY | 164 | 42.570 | 74.911 | 9.560 | 1.00 | 27.71 | B_13 |
| ATOM | 3013 | ZN | ZN | 166 | 51.961 | 60.891 | -2.865 | 1.00 | 28.31 | BION |
| ATOM | 3014 | ZN | ZN | 167 | 56.468 | 50.981 | 3.458 | 1.00 | 26.20 | BION |
| ATOM | 3015 | CA | CA | 168 | 63.096 | 53.752 | -5.445 | 1.00 | 14.89 | BION |
| ATOM | 3016 | CA | CA | 165 | 50.705 | 55.618 | 13.085 | 1.00 | 15.79 | BION |
| ATOM | 3047 | C5 | WAY | 169 | 54.585 | 56.119 | -6.288 | 1.00 | 40.09 | B693 |
| ATOM | 3048 | CF1 | WAY | 169 | 54.019 | 54.934 | -5.802 | 1.00 | 21.52 | B693 |
| ATOM | 3049 | CH | WAY | 169 | 53.271 | 54.923 | -4.624 | 1.00 | 32.32 | B693 |
| ATOM | 3050 | C2 | WAY | 169 | 53.100 | 56.104 | -3.898 | 1.00 | 21.39 | B693 |
| ATOM | 3051 | C3 | WAY | 169 | 53.667 | 57.286 | -4.369 | 1.00 | 18.26 | B693 |
| ATOM | 3052 | C4 | WAY | 169 | 54.402 | 57.308 | -5.540 | 1.00 | 20.63 | B693 |
| ATOM | 3053 | N20 | WAY | 169 | 54.933 | 58.531 | -5.964 | 1.00 | 22.15 | B693 |
| ATOM | 3054 | CD | WAY | 169 | 54.297 | 59.340 | -7.031 | 1.00 | 30.92 | B693 |
| ATOM | 3055 | C23 | WAY | 169 | 53.576 | 58.491 | -8.087 | 1.00 | 20.75 | B693 |
| ATOM | 3056 | C28 | WAY | 169 | 54.224 | 58.114 | -9.279 | 1.00 | 34.14 | B693 |
| ATOM | 3057 | C27 | WAY | 169 | 53.539 | 57.335 | -10.228 | 1.00 | 33.99 | B693 |
| ATOM | 3058 | CM | WAY | 169 | 52.209 | 56.944 | -9.968 | 1.00 | 23.49 | B693 |
| ATOM | 3059 | N25 | WAY | 169 | 51.602 | 57.318 | -8.814 | 1.00 | 23.61 | B693 |
| ATOM | 3060 | C24 | WAY | 169 | 52.246 | 58.071 | -7.880 | 1.00 | 20.52 | B693 |
| ATOM | 3061 | S21 | WAY | 169 | 56.531 | 58.783 | -5.660 | 1.00 | 20.46 | B693 |
| ATOM | 3062 | C16 | WAY | 169 | 56.457 | 60.446 | -5.010 | 1.00 | 39.00 | B693 |
| ATOM | 3063 | C21 | WAY | 169 | 56.700 | 60.669 | -3.634 | 1.00 | 28.79 | B693 |
| ATOM | 3064 | C20 | WAY | 169 | 56.656 | 61.967 | -3.109 | 1.00 | 12.65 | B693 |
| ATOM | 3065 | C19 | WAY | 169 | 56.373 | 63.058 | -3.946 | 1.00 | 15.68 | B693 |
| ATOM | 3066 | C18 | WAY | 169 | 56.126 | 62.828 | -5.319 | 1.00 | 12.08 | B693 |
| ATOM | 3067 | C17 | WAY | 169 | 56.169 | 61.538 | -5.852 | 1.00 | 15.19 | B693 |
| ATOM | 3068 | O33 | WAY | 169 | 56.337 | 64.360 | -3.424 | 1.00 | 16.79 | B693 |
| ATOM | 3069 | C36 | WAY | 169 | 56.982 | 65.456 | -4.084 | 1.00 | 20.80 | B693 |
| ATOM | 3070 | O15 | WAY | 169 | 56.973 | 57.923 | -4.580 | 1.00 | 21.90 | B693 |
| ATOM | 3071 | O14 | WAY | 169 | 57.259 | 58.799 | -6.913 | 1.00 | 10.86 | B693 |
| ATOM | 3072 | C7 | WAY | 169 | 53.486 | 58.556 | -3.613 | 1.00 | 10.00 | B693 |
| ATOM | 3073 | N9 | WAY | 169 | 53.741 | 58.606 | -2.303 | 1.00 | 10.00 | B693 |
| ATOM | 3074 | O10 | WAY | 169 | 53.539 | 59.846 | -1.659 | 1.00 | 23.73 | B693 |
| ATOM | 3075 | O8 | WAY | 169 | 53.107 | 59.569 | -4.154 | 1.00 | 15.89 | B693 |
| ATOM | 3076 | C29 | WAY | 169 | 55.383 | 55.968 | -7.606 | 1.00 | 28.30 | B693 |
| ATOM | 1 | OH2 | WAT | 301 | 67.399 | 53.332 | 19.612 | 1.00 | 10.00 | SOLV |
| ATOM | 2 | OH2 | WAT | 302 | 61.288 | 46.506 | 17.898 | 1.00 | 10.00 | SOLV |
| ATOM | 3 | OH2 | WAT | 303 | 79.538 | 50.433 | 20.115 | 1.00 | 10.00 | SOLV |
| ATOM | 4 | OH2 | WAT | 304 | 80.982 | 25.236 | 19.076 | 1.00 | 26.37 | SOLV |
| ATOM | 5 | OH2 | WAT | 305 | 82.461 | 30.767 | 19.346 | 1.00 | 13.02 | SOLV |
| ATOM | 6 | OH2 | WAT | 306 | 67.759 | 41.912 | 4.887 | 1.00 | 17.30 | SOLV |
| ATOM | 7 | OH2 | WAT | 307 | 60.785 | 41.727 | 10.585 | 1.00 | 20.42 | SOLV |
| ATOM | 8 | OH2 | WAT | 308 | 89.638 | 33.523 | 25.640 | 1.00 | 33.45 | SOLV |
| ATOM | 9 | OH2 | WAT | 309 | 77.721 | 51.975 | 4.391 | 1.00 | 13.91 | SOLV |
| ATOM | 10 | OH2 | WAT | 310 | 96.022 | 34.702 | 6.692 | 1.00 | 25.50 | SOLV |
| ATOM | 11 | OH2 | WAT | 311 | 71.292 | 38.746 | 26.741 | 1.00 | 13.06 | SOLV |
| ATOM | 12 | OH2 | WAT | 312 | 85.939 | 49.781 | 3.498 | 1.00 | 12.04 | SOLV |
| ATOM | 13 | OH2 | WAT | 313 | 58.101 | 41.127 | 10.261 | 1.00 | 40.97 | SOLV |
| ATOM | 14 | OH2 | WAT | 314 | 86.373 | 42.692 | 0.747 | 1.00 | 17.24 | SOLV |
| ATOM | 15 | OH2 | WAT | 315 | 78.257 | 39.885 | 24.626 | 1.00 | 18.57 | SOLV |
| ATOM | 16 | OH2 | WAT | 316 | 68.341 | 48.572 | 25.558 | 1.00 | 18.33 | SOLV |
| ATOM | 17 | OH2 | WAT | 317 | 79.806 | 29.147 | 18.371 | 1.00 | 10.00 | SOLV |
| ATOM | 18 | OH2 | WAT | 318 | 87.119 | 44.480 | 23.137 | 1.00 | 46.31 | SOLV |
| ATOM | 19 | OH2 | WAT | 319 | 55.885 | 39.688 | 11.459 | 1.00 | 21.26 | SOLV |
| ATOM | 20 | OH2 | WAT | 320 | 73.250 | 41.084 | 0.386 | 1.00 | 18.49 | SOLV |
| ATOM | 21 | OH2 | WAT | 321 | 72.079 | 46.488 | -6.835 | 1.00 | 27.48 | SOLV |
| ATOM | 22 | OH2 | WAT | 322 | 71.923 | 37.638 | -3.750 | 1.00 | 29.19 | SOLV |
| ATOM | 23 | OH2 | WAT | 323 | 74.998 | 28.451 | 2.684 | 1.00 | 34.60 | SOLV |
| ATOM | 24 | OH2 | WAT | 324 | 87.769 | 44.123 | 9.214 | 1.00 | 15.60 | SOLV |
| ATOM | 25 | OH2 | WAT | 325 | 86.113 | 24.382 | 16.709 | 1.00 | 25.17 | SOLV |
| ATOM | 26 | OH2 | WAT | 326 | 81.205 | 57.603 | 0.529 | 1.00 | 34.27 | SOLV |
| ATOM | 27 | OH2 | WAT | 327 | 75.163 | 62.739 | 12.391 | 1.00 | 16.47 | SOLV |
| ATOM | 28 | OH2 | WAT | 328 | 65.604 | 44.690 | 2.830 | 1.00 | 26.64 | SOLV |
| ATOM | 29 | OH2 | WAT | 329 | 61.899 | 45.512 | 29.269 | 1.00 | 15.82 | SOLV |
| ATOM | 30 | OH2 | WAT | 330 | 58.763 | 41.730 | 8.338 | 1.00 | 27.95 | SOLV |
| ATOM | 31 | OH2 | WAT | 331 | 69.823 | 44.729 | 6.258 | 1.00 | 13.37 | SOLV |
| ATOM | 32 | OH2 | WAT | 332 | 79.220 | 61.263 | 12.781 | 1.00 | 28.84 | SOLV |
| ATOM | 33 | OH2 | WAT | 333 | 78.105 | 37.095 | 27.911 | 1.00 | 34.48 | SOLV |
| ATOM | 34 | OH2 | WAT | 334 | 75.939 | 25.608 | 12.364 | 1.00 | 35.21 | SOLV |
| ATOM | 35 | OH2 | WAT | 335 | 90.256 | 42.668 | 16.539 | 1.00 | 45.05 | SOLV |
| ATOM | 36 | OH2 | WAT | 336 | 86.761 | 51.457 | 13.881 | 1.00 | 25.26 | SOLV |
| ATOM | 37 | OH2 | WAT | 337 | 67.479 | 42.004 | -5.009 | 1.00 | 33.30 | SOLV |
| ATOM | 38 | OH2 | WAT | 338 | 82.018 | 50.963 | 8.823 | 1.00 | 19.80 | SOLV |
| ATOM | 39 | OH2 | WAT | 339 | 80.278 | 32.895 | -1.126 | 1.00 | 30.16 | SOLV |
| ATOM | 40 | OH2 | WAT | 340 | 71.683 | 50.944 | 31.567 | 1.00 | 29.62 | SOLV |

71/75

| | | | | | | | | | | |
|------|-----|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 41 | OH2 | WAT | 341 | 61.633 | 49.360 | 10.951 | 1.00 | 15.47 | SOLV |
| ATOM | 42 | OH2 | WAT | 342 | 89.589 | 43.811 | 5.959 | 1.00 | 18.08 | SOLV |
| ATOM | 43 | OH2 | WAT | 343 | 70.742 | 35.952 | 14.932 | 1.00 | 34.03 | SOLV |
| ATOM | 44 | OH2 | WAT | 344 | 89.836 | 28.590 | 26.657 | 1.00 | 18.11 | SOLV |
| ATOM | 45 | OH2 | WAT | 345 | 70.822 | 32.764 | 1.461 | 1.00 | 22.35 | SOLV |
| ATOM | 46 | OH2 | WAT | 346 | 63.056 | 34.653 | 0.491 | 1.00 | 29.51 | SOLV |
| ATOM | 47 | OH2 | WAT | 347 | 58.054 | 46.282 | 2.363 | 1.00 | 10.00 | SOLV |
| ATOM | 48 | OH2 | WAT | 348 | 67.914 | 58.660 | -6.267 | 1.00 | 18.30 | SOLV |
| ATOM | 49 | OH2 | WAT | 349 | 70.170 | 56.725 | 0.575 | 1.00 | 11.89 | SOLV |
| ATOM | 50 | OH2 | WAT | 350 | 55.922 | 73.897 | 0.623 | 1.00 | 18.86 | SOLV |
| ATOM | 51 | OH2 | WAT | 351 | 73.489 | 53.195 | 2.061 | 1.00 | 24.35 | SOLV |
| ATOM | 52 | OH2 | WAT | 352 | 58.033 | 50.530 | 19.075 | 1.00 | 25.52 | SOLV |
| ATOM | 53 | OH2 | WAT | 353 | 63.245 | 57.302 | 17.340 | 1.00 | 13.88 | SOLV |
| ATOM | 54 | OH2 | WAT | 354 | 58.442 | 71.334 | -5.670 | 1.00 | 17.51 | SOLV |
| ATOM | 55 | OH2 | WAT | 355 | 62.535 | 61.154 | 16.706 | 1.00 | 12.38 | SOLV |
| ATOM | 56 | OH2 | WAT | 356 | 66.949 | 51.163 | -10.284 | 1.00 | 17.92 | SOLV |
| ATOM | 57 | OH2 | WAT | 357 | 57.588 | 54.191 | 9.850 | 1.00 | 17.88 | SOLV |
| ATOM | 58 | OH2 | WAT | 358 | 64.836 | 48.085 | 4.627 | 1.00 | 17.80 | SOLV |
| ATOM | 59 | OH2 | WAT | 359 | 66.445 | 61.785 | 19.640 | 1.00 | 24.12 | SOLV |
| ATOM | 60 | OH2 | WAT | 360 | 55.740 | 42.557 | 0.533 | 1.00 | 27.32 | SOLV |
| ATOM | 61 | OH2 | WAT | 361 | 74.075 | 57.146 | 13.179 | 1.00 | 18.01 | SOLV |
| ATOM | 62 | OH2 | WAT | 362 | 46.987 | 69.315 | -2.545 | 1.00 | 11.87 | SOLV |
| ATOM | 63 | OH2 | WAT | 363 | 53.842 | 52.266 | -2.612 | 1.00 | 25.20 | SOLV |
| ATOM | 64 | OH2 | WAT | 364 | 33.425 | 65.313 | -4.686 | 1.00 | 28.97 | SOLV |
| ATOM | 65 | OH2 | WAT | 365 | 45.633 | 51.173 | 10.502 | 1.00 | 31.97 | SOLV |
| ATOM | 66 | OH2 | WAT | 366 | 39.040 | 71.050 | -0.722 | 1.00 | 20.81 | SOLV |
| ATOM | 67 | OH2 | WAT | 367 | 54.517 | 67.335 | -6.251 | 1.00 | 46.24 | SOLV |
| ATOM | 68 | OH2 | WAT | 368 | 45.083 | 67.138 | 20.314 | 1.00 | 29.47 | SOLV |
| ATOM | 69 | OH2 | WAT | 369 | 65.758 | 67.669 | -6.655 | 1.00 | 14.69 | SOLV |
| ATOM | 70 | OH2 | WAT | 370 | 44.943 | 78.174 | 12.948 | 1.00 | 23.88 | SOLV |
| ATOM | 71 | OH2 | WAT | 371 | 37.141 | 57.403 | 1.723 | 1.00 | 23.72 | SOLV |
| ATOM | 72 | OH2 | WAT | 372 | 62.407 | 66.806 | 13.368 | 1.00 | 13.36 | SOLV |
| ATOM | 73 | OH2 | WAT | 373 | 50.776 | 47.263 | 5.661 | 1.00 | 38.22 | SOLV |
| ATOM | 74 | OH2 | WAT | 374 | 56.697 | 47.264 | 11.752 | 1.00 | 24.75 | SOLV |
| ATOM | 75 | OH2 | WAT | 375 | 42.566 | 60.884 | 15.739 | 1.00 | 16.25 | SOLV |
| ATOM | 76 | OH2 | WAT | 376 | 59.299 | 74.342 | 13.838 | 1.00 | 31.27 | SOLV |
| ATOM | 77 | OH2 | WAT | 377 | 72.976 | 63.691 | -0.667 | 1.00 | 20.36 | SOLV |
| ATOM | 78 | OH2 | WAT | 378 | 72.876 | 60.516 | -6.752 | 1.00 | 34.24 | SOLV |
| ATOM | 79 | OH2 | WAT | 379 | 63.998 | 68.760 | 16.371 | 1.00 | 19.04 | SOLV |
| ATOM | 80 | OH2 | WAT | 380 | 44.947 | 66.728 | -2.566 | 1.00 | 29.51 | SOLV |
| ATOM | 81 | OH2 | WAT | 381 | 57.690 | 61.926 | -9.414 | 1.00 | 29.01 | SOLV |
| ATOM | 82 | OH2 | WAT | 382 | 44.595 | 80.810 | 5.831 | 1.00 | 27.43 | SOLV |
| ATOM | 83 | OH2 | WAT | 383 | 78.065 | 36.583 | 24.121 | 1.00 | 14.08 | SOLV |
| ATOM | 84 | OH2 | WAT | 384 | 42.289 | 64.651 | -0.868 | 1.00 | 25.57 | SOLV |
| ATOM | 85 | OH2 | WAT | 385 | 59.851 | 68.458 | -12.381 | 1.00 | 30.18 | SOLV |
| ATOM | 86 | OH2 | WAT | 386 | 53.784 | 72.644 | -4.782 | 1.00 | 22.35 | SOLV |
| ATOM | 87 | OH2 | WAT | 387 | 72.793 | 27.922 | 8.925 | 1.00 | 32.13 | SOLV |
| ATOM | 88 | OH2 | WAT | 388 | 57.224 | 68.062 | -6.072 | 1.00 | 17.87 | SOLV |
| ATOM | 89 | OH2 | WAT | 389 | 45.210 | 44.988 | 4.285 | 1.00 | 25.10 | SOLV |
| ATOM | 90 | OH2 | WAT | 390 | 49.413 | 53.782 | 1.546 | 1.00 | 21.68 | SOLV |
| ATOM | 91 | OH2 | WAT | 391 | 45.232 | 59.677 | 1.393 | 1.00 | 19.25 | SOLV |
| ATOM | 92 | OH2 | WAT | 392 | 42.551 | 59.954 | 5.056 | 1.00 | 27.30 | SOLV |
| ATOM | 93 | OH2 | WAT | 393 | 58.412 | 43.750 | 3.948 | 1.00 | 58.70 | SOLV |
| ATOM | 94 | OH2 | WAT | 394 | 56.942 | 54.199 | -2.588 | 1.00 | 31.14 | SOLV |
| ATOM | 95 | OH2 | WAT | 395 | 55.216 | 51.994 | 9.824 | 1.00 | 13.25 | SOLV |
| ATOM | 96 | OH2 | WAT | 396 | 51.642 | 54.651 | 14.874 | 1.00 | 10.00 | SOLV |
| ATOM | 97 | OH2 | WAT | 397 | 48.690 | 56.156 | 13.991 | 1.00 | 28.59 | SOLV |
| ATOM | 98 | OH2 | WAT | 398 | 74.412 | 37.913 | 0.396 | 1.00 | 12.55 | SOLV |
| ATOM | 99 | OH2 | WAT | 399 | 81.920 | 53.968 | 18.267 | 1.00 | 14.05 | SOLV |
| ATOM | 100 | OH2 | WAT | 400 | 70.413 | 41.780 | 1.170 | 1.00 | 16.68 | SOLV |
| ATOM | 101 | OH2 | WAT | 401 | 71.098 | 53.544 | 2.407 | 1.00 | 27.63 | SOLV |
| ATOM | 102 | OH2 | WAT | 402 | 94.383 | 32.979 | 9.497 | 1.00 | 27.97 | SOLV |
| ATOM | 103 | OH2 | WAT | 403 | 70.765 | 66.069 | 16.389 | 1.00 | 38.09 | SOLV |
| ATOM | 104 | OH2 | WAT | 404 | 78.651 | 34.890 | 29.495 | 1.00 | 48.60 | SOLV |
| ATOM | 105 | OH2 | WAT | 405 | 80.289 | 39.811 | 24.727 | 1.00 | 20.74 | SOLV |
| ATOM | 106 | OH2 | WAT | 406 | 63.627 | 47.414 | 7.301 | 1.00 | 40.21 | SOLV |
| ATOM | 107 | OH2 | WAT | 407 | 74.679 | 30.772 | 11.524 | 1.00 | 37.03 | SOLV |
| ATOM | 108 | OH2 | WAT | 408 | 80.240 | 36.041 | 26.681 | 1.00 | 27.42 | SOLV |
| ATOM | 109 | OH2 | WAT | 409 | 84.971 | 25.909 | 18.426 | 1.00 | 24.96 | SOLV |
| ATOM | 110 | OH2 | WAT | 410 | 57.832 | 41.294 | 5.792 | 1.00 | 71.90 | SOLV |
| ATOM | 111 | OH2 | WAT | 411 | 55.484 | 68.139 | -9.086 | 1.00 | 48.47 | SOLV |
| ATOM | 112 | OH2 | WAT | 412 | 65.535 | 68.260 | 2.400 | 1.00 | 26.24 | SOLV |
| ATOM | 113 | OH2 | WAT | 413 | 80.085 | 42.291 | -3.144 | 1.00 | 26.49 | SOLV |
| ATOM | 114 | OH2 | WAT | 414 | 82.088 | 37.456 | 27.733 | 1.00 | 42.54 | SOLV |
| ATOM | 115 | OH2 | WAT | 415 | 61.020 | 53.195 | 21.566 | 1.00 | 38.16 | SOLV |
| ATOM | 116 | OH2 | WAT | 416 | 55.968 | 70.365 | -5.096 | 1.00 | 28.42 | SOLV |
| ATOM | 117 | OH2 | WAT | 417 | 51.619 | 57.620 | -0.487 | 1.00 | 41.81 | SOLV |

72 / 75

| | | | | | | | | | | |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 118 | OH2 | WAT | 418 | 40.651 | 66.108 | 2.086 | 1.00 | 40.11 | SOLV |
| ATOM | 119 | OH2 | WAT | 419 | 58.453 | 49.818 | 7.926 | 1.00 | 38.96 | SOLV |
| ATOM | 120 | OH2 | WAT | 420 | 53.768 | 51.716 | 13.623 | 1.00 | 43.62 | SOLV |
| ATOM | 121 | OH2 | WAT | 421 | 76.068 | 60.373 | 21.292 | 1.00 | 39.30 | SOLV |
| ATOM | 122 | OH2 | WAT | 422 | 56.186 | 50.034 | 17.422 | 1.00 | 37.47 | SOLV |
| END | | | | | | | | | | |

73/75

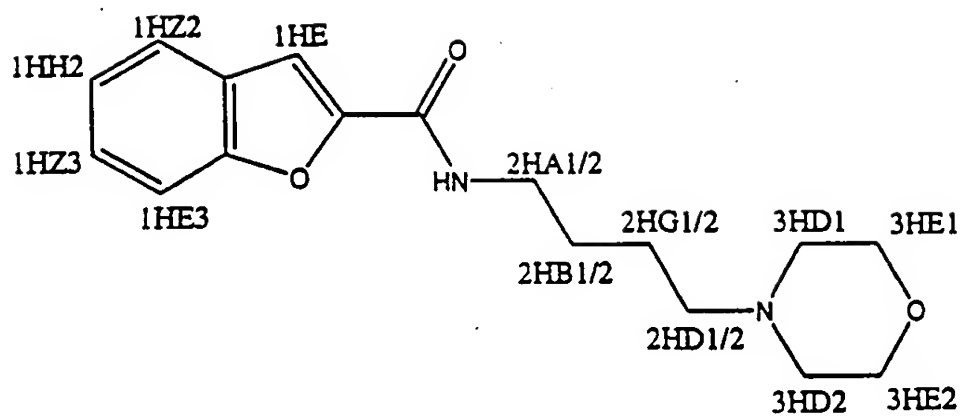


FIG. 6

74/75

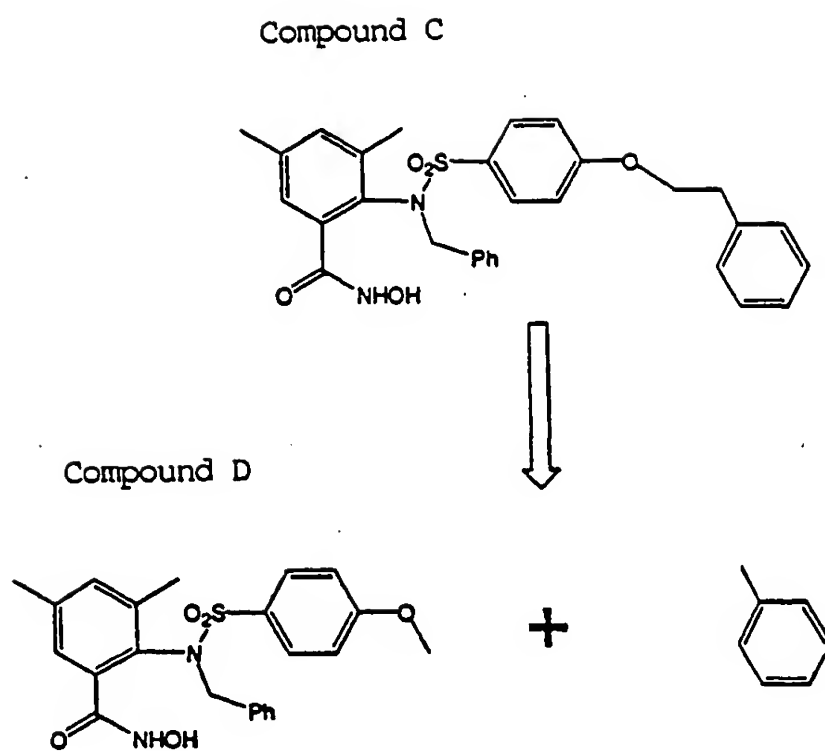
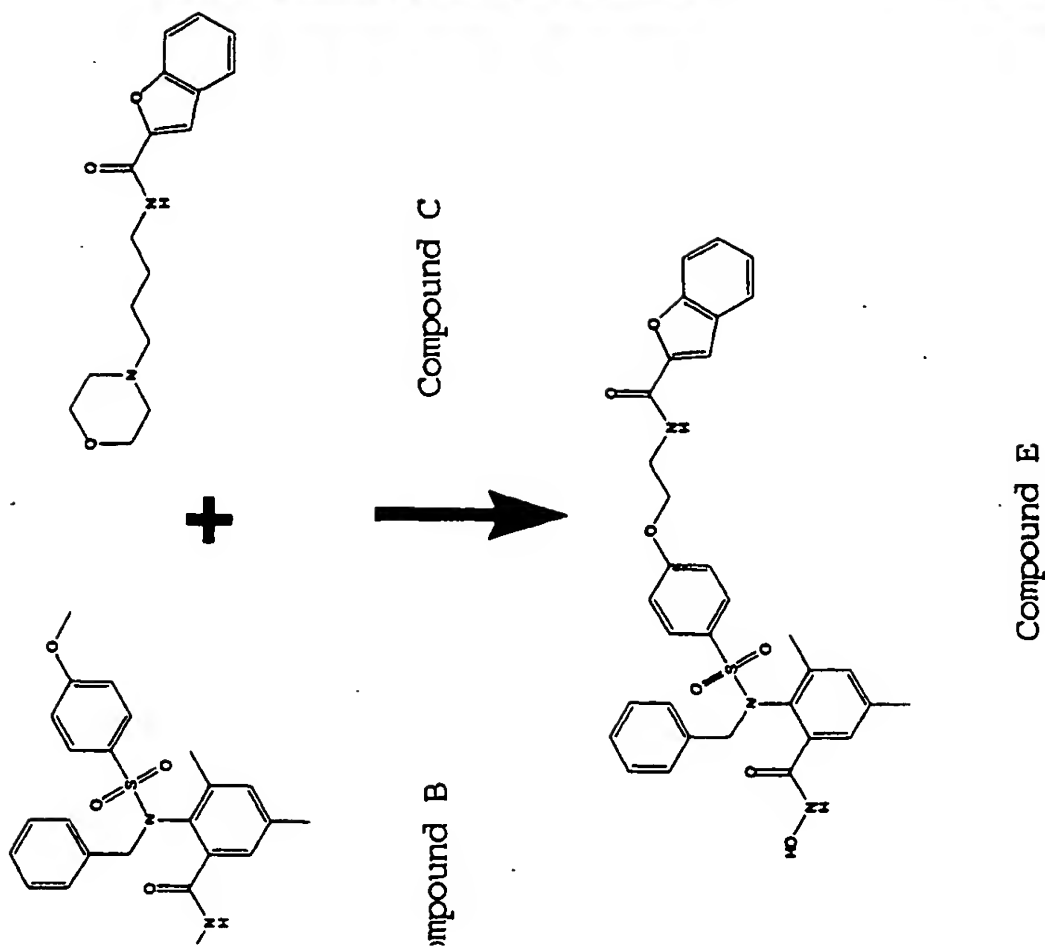


FIG. 7

75 / 75



FIG. 8



INTERNATIONAL SEARCH REPORT

International application No.

PCT/US01/05150

A. * CLASSIFICATION OF SUBJECT MATTER

IPC(7) : G01N 9/00, 33/48

US CL : 435/183; 702/22

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 435/183; 702/22

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched
NONEElectronic data base consulted during the international search (name of data base and, where practicable, search terms used)
STN: WEST

C. DOCUMENTS CONSIDERED TO BE RELEVANT

| Category* | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|-----------|--|-----------------------|
| X | GOMIS-RUTH, F.X. et al. The helping hand of collagenase-3 (MMP-13: 2.7, ANG> crystal structure of its C-terminal haemopexin-like domain. Journal Mol. Biol. 1996, Vol. 264, No. 3, pages 556-566, see entire document. | 8-14 |
| X | US 6,008,243 A (BENDER et al.) 28 December 1999(28.12.99), see entire document. | 1-7, 15-20 |

☐ Further documents are listed in the continuation of Box C. ☐ See patent family annex.

| | |
|---|--|
| * Special categories of cited documents: | *T* later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention |
| *A* document defining the general state of the art which is not considered to be of particular relevance | *X* document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone |
| *B* earlier document published on or after the international filing date | *Y* document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art |
| *L* document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified) | *Z* document member of the same patent family |
| *O* document referring to an oral disclosure, use, exhibition or other means | |
| *P* document published prior to the international filing date but later than the priority date claimed | |

Date of the actual completion of the international search

12 JULY 2001

Date of mailing of the international search report

30 JUL 2001

Name and mailing address of the ISA/US
Commissioner of Patents and Trademarks
Box PCT
Washington, D.C. 20231

Facsimile No. (703) 305-3230

Authorized official
Rosetta Laurence For
AMY J. HARTTER

Telephone No. (703) 308-0196

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:
2. ☐ Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:
3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

Please See Extra Sheet.

1. ☒ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

☐

The additional search fees were accompanied by the applicant's protest.

☐

No protest accompanied the payment of additional search fees.

BOX II. OBSERVATIONS WHERE UNITY OF INVENTION WAS LACKING

This ISA found multiple inventions as follows:

This application contains the following inventions or groups of inventions which are not so linked as to form a single inventive concept under PCT Rule 13.1. In order for these inventions to be searched the appropriate search fees must be paid.

Group I which consists of claims 1-7 is distinct as it addresses itself to the solution complex of the mixture of MMP-13 and the defined "Compound A." The solution is clearly distinct and different from the crystal complex, active site and methods that are claimed in succeeding groups and according claims.

Group II consists of claims 8-14. These claims pertain to the actual product of the crystal complex in its entirety. Thus it is distinct from Groups I and Groups 3-4. The group claims the whole crystal known as "Compound A" and the crystal is not in any other type of alternate environment or with any additional accoutrements.

Group III encompasses the claims of 15-20. These claims consist of the active site of the molecule of MMP-13. This chemical is a portion of the solution claimed in the first group and thus separate and distinct from the solution of Group I or the separate entity of "Compound A" that is claimed in Group 2. Thus these Groups are separate.

Group IV consists of claims 21-32 which claim a method of identifying an inhibitor or activator of the MMP-13 compound. The method that is embodied within this Group is clearly different from the preceding groups. Firstly the claims within Group 4 are directed toward a method of accomplishing the task of identifying different entities and not a product itself. Secondly its actions are addressed to entities outside the compound itself and not limited to "Compound A" of the MMP-13. Based on the aforementioned reasons and the distinct nature of the claims defined in each of the groups, the instant application has a lack of unity due to each group having a different Special Technical Feature as summarized above for each group.

THIS PAGE BLANK (USPTO)